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# Predicting and Forecasting Surface Water Acidification A Plan for Assessing Data Aggregation Effects

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# PREDICTING AND FORECASTING SURFACE WATER ACIDIFICATION: A PLAN FOR ASSESSING DATA AGGREGATION EFFECTS

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16. ABSTRACT

A major goal of the Direct/Delayed Response Project (DDRP), a project within the U. S. Environmental Protection Agency's(EPA) Aquatic Effects Research Program (AERP) is to project potential changes in surface water chemistry in lakes in the northeastern U. S. and streams in the Mid-Appalachians and southeastern U. S., over the next 50 years as a function of current and alternative levels of acidic deposition. The DDRP projection are based on various types of simulations models that predict surface water and soil chemistry. All models- statistical, empirical, mechanistic, logical or others - represent a simplification or abstraction of the real world. A major question associated with the application of an model is how to prepare subset, and aggregate, or lump, data so that they will represent the processes and system being simulated.

The models used in the DDRP require physical and chemical data on watershed soils as part of the model inputs. In conjunction with the DDRP, soil surveys were conducted in selected watersheds in each of the three regions. This document describes and discusses the approaches used in the DDRP for aggregating soil chemical and physical data for use in the various DDRP analyses.

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## PREFACE

This document has been prepared by scientists working on the EPA's Direct/Delayed Response Project (DDRP). It describes the rationale and methodology developed in the course of the DDRP for combining, or aggregating, soil physical and chemical data to reduce the amount of data required to numerically represent watershed characteristics with minimal loss of information and to insure that the aggregated data effectively represent watershed characteristics. The aggregated data were used in statistical analyses and computer simulation models to make regional assessments of the effects of acidic deposition on soils and surface water.

Although not all of the analyses discussed in this document have been completed, we believe the document contains information that will be useful to scientists faced with using large, regional, environmental datasets for regional assessments. It should also be useful to scientists working at a variety of spatial scales, since it describes how to collect data at one scale for use at another.

# SECTION 1

# INTRODUCTION

## 1.1 PURPOSE

A major goal of the Direct/Delayed Response Project (DDRP) (Church, 1989; Church et al., 1990), a project within the U.S. Environmental Protection Agency's (EPA) Aquatic Effects Research Program (AERP), is to project potential changes in surface water chemistry in lakes in the northeastern United States and streams in the Mid-Appalachians and southeastern United States, over the next 50 years as a function of current and alternative levels of acidic deposition. The DDRP projection are based on various types of simulations models that predict surface water and soil chemistry. All models -- statistical, empirical, mechanistic, logical or others -- represent a simplification or abstraction of the real world. A major question associated with the application of any model is how to prepare, subset, and aggregate, or lump, data so that they will represent the processes and system being simulated.

The models used in the DDRP require physical and chemical data on watershed soils as part of the model inputs. In conjunction with the DDRP, soil surveys were conducted in selected watersheds in each of the three regions (Lee et al., 1989a). Soil samples were collected from individual horizons within pedons in these watersheds. The focus of the DDRP, however, is on regional responses to acidic deposition, not individual soil sample or pedon response. To evaluate watershed response using the various types of models in DDRP, these distributed data had to be aggregated, averaged, or combined in some fashion to represent or describe the watersheds. This document describes and discusses the approaches used in the DDRP for aggregating soil chemical and physical data for use in the various DDRP analyses. The intended audience is both the scientific and administrative communities interested in (1) the approaches to aggregation of large datasets, and (2) the specific procedures used in the DDRP.

## 1.2 BACKGROUND

In 1983, the EPA, in conjunction with the National Acid Precipitation Assessment Program (NAPAP), established the Aquatic Effects Research Program (AERP) to assess and evaluate the effects of acidic deposition on aquatic resources. The AERP focuses on four environmental policy questions:

1. What is the extent and magnitude of past change in aquatic resources that is attributable to acidic deposition?
2. What change is expected in the future under various deposition scenarios?

3. What is the target loading of sulfate below which changes would not be expected?
4. What will be the rate and extent of recovery if sulfate deposition decreases?

In each instance, the answers to these questions are to be regional in scale, and the results are to be expressed with quantitative estimates of uncertainty.

The primary purpose of the AERP is to address the policy and assessment questions listed above through (1) assessing the current chemical status and extent of aquatic systems potentially at risk because of acidic deposition and (2) Understanding and predicting the future effects of acidic deposition on these aquatic resources.

A concurrent objective of AERP is to identify scientific uncertainties that affect potential answers to these assessment or policy questions.

### 1.3 AERP COMPONENTS

The primary component projects within the AERP are the National Surface Water Survey (NSWS), the Direct/Delayed Response Project (DDRP), the Watershed Manipulation Project (WMP), and the Episodic Response Project (ERP). These projects collectively encompass three major elements of the assessment questions:

1. Quantification of the chemical status and extent of surface waters at risk (NSWS, ERP);
2. Prediction of the future chemical and biological changes within aquatic ecosystems (DDRP, ERP);
3. Verification of these predictions and development of an improved understanding of controlling mechanisms (WMP, ERP); and
4. Corroboration or validation of these findings through long-term monitoring (TIME).

Four of the projects focused on chronic acidification; the ERP was designed, however, to address the same questions by examining the effects of episodic acidification that result from storm and snowmelt events. The NSWS (Linthurst et al., 1986; Landers et al., 1987; Kaufmann et al., 1988) was designed within a statistical frame and permits quantitative estimates of the numbers and percentages of acidic lakes or streams in regions of the United States considered to be potentially sensitive to acidic deposition (Figure 1-1). The NSWS regions and subregions, studied as part of the Survey, form the foundation of the AERP. Surveys of fall chemistry in lakes confirmed the presence of acidic systems, whose waters had no acid neutralizing capacity (i.e., ANC was $\leq 0$ $\mu$eq/L), in the Northeast, the Upper Midwest, and Florida. No acidic lakes were found in the Southern Blue Ridge Province (SBRP) or the West. Surveys of spring runoff in streams focused on regions that contain few natural lakes. The National Stream Survey (NSS) (Kaufmann et al., 1988) showed that acidic surface waters extended as far south as West Virginia and Virginia in the Mid-Atlantic region, but not into the

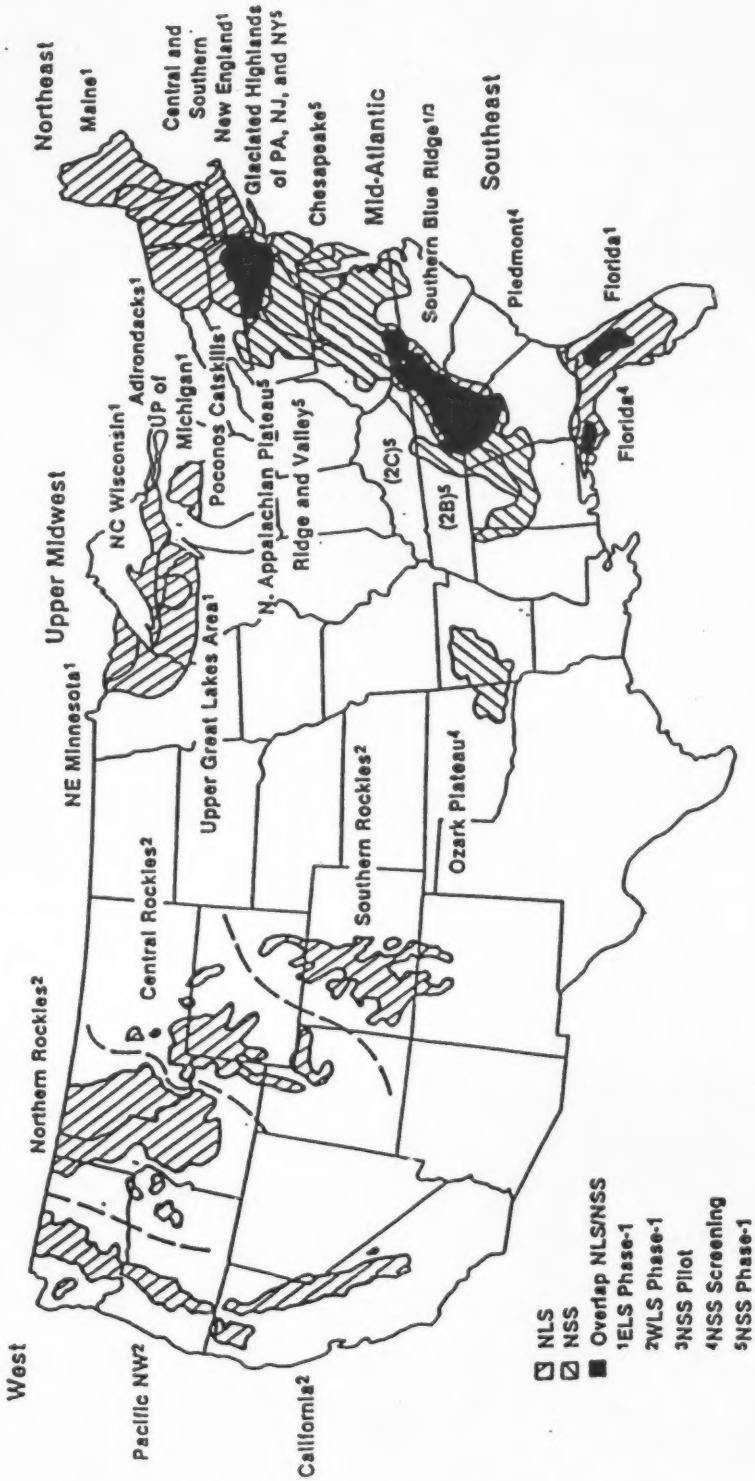


Figure 1-1. Regions and subregions of the United States used to define target populations for the National Surface Water Survey.

Southeastern Appalachians or the Piedmont. With an estimate of the current regional status of lakes and streams, the next important question is how many of these lakes and streams, not currently acidic, might become acidic in the future at current and changing levels of acidic deposition. The AERP designed and implemented a research program to project the future response of watersheds and surface waters to acidic deposition. This research program is known as the Direct/Delayed Response Project (DDRP) (Church, 1989).

### 1.4 DDRP

The DDRP was designed to forecast the change in surface water chemistry over the next 50 years for lakes in the Northeast (NE) and streams in the Mid-Appalachians (M-APP) and in the Southern Blue Ridge Province (SBRP) (Figure 1-2), assuming current and alternative levels of deposition. Particular emphasis is on the number of lakes and streams that might become acidic (i.e., ANC $\leq$ 0) at various levels of deposition over the next 50 years.

In defining the regions of concern, the intent was to focus on regions with watersheds potentially susceptible to acidic deposition, yet exhibiting a wide contrast in both soil and watershed characteristics and levels of deposition. The contrast in watershed characteristics and levels of deposition was included to maximize the probability of successfully identifying the processes most important in determining watershed response. Certain regions of the United States contain an abundance of low ANC waters and, therefore, are potentially susceptible to acidic deposition.

The DDRP focused on the northeastern United States, the upland areas of Mid-Appalachia, and a mountainous section of the southeast, commonly called the Southern Blue Ridge Province. The Northeast currently has acidic lakes and the question is whether additional lakes might become acidic in the future at current or altered levels of sulfur deposition. A second question is whether currently acidic lakes might recover under decreased deposition rates. In contrast, deposition is increasing in the Southeast and the full effects of acidic deposition may not be realized for some time, due to sulfate retention in watershed soils. The question in the Southeast is whether stream systems might become acidic in the future at current or alternative levels of deposition.

#### 1.4.1 DDRP Objectives

The DDRP has four primary objectives:

1. to describe the regional variability of soil and watershed characteristics;
2. to determine which soil and watershed characteristics are most strongly related to surface water chemistry;

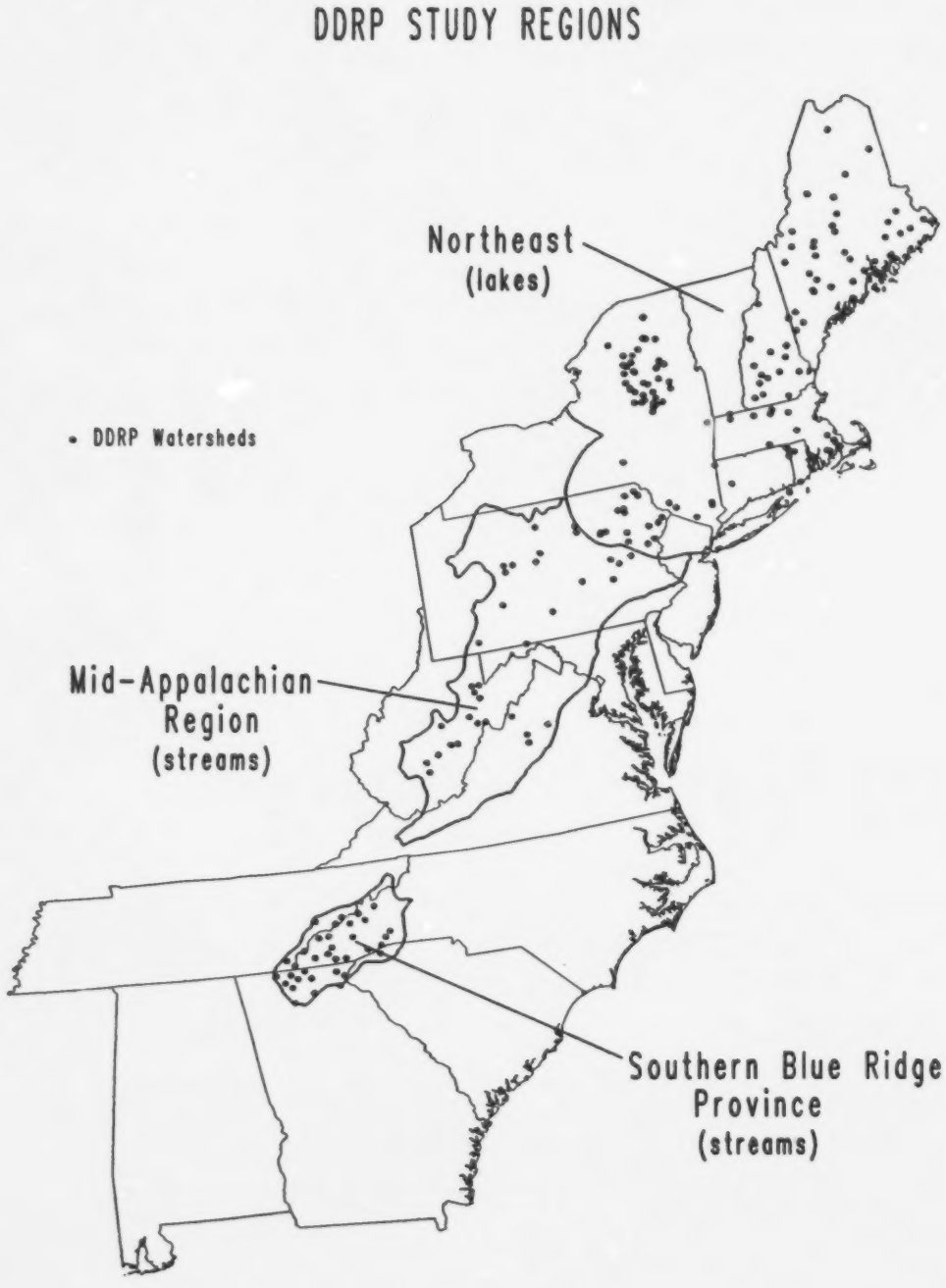


Figure 1-2. DDRP regions of study: the Northeast, the Mid-Appalachians, and the Southern Blue Ridge Province.

3. to estimate the relative importance of key watershed processes in moderating regional effects of acidic deposition; and
4. to classify a sample of watersheds with regard to their response characteristics to inputs of acidic deposition and to extrapolate the results from the sample of watersheds to the target population of systems in the regions of concern.

The DDRP employed a variety of methods to accomplish its objectives. Three levels of analysis, designated as Levels I, II, and III, were used to analyze the soil survey and sample data, and to classify the watershed response to acidic deposition. The following paragraphs briefly describe the soil survey and the three levels of analysis.

### 1.4.2 DDRP Components

#### 1.4.2.1 Soil Surveys

The soil surveys were designed to address the first DDRP objective, characterizing the physical and chemical variability of watershed soils across the NE, M-APP, and SBRP (Lee et al., 1989a). The first soil survey was conducted in fall 1985 on 145 northeastern watersheds selected in conjunction with Phase II of the Eastern Lake Survey (ELS). The second soil survey was conducted in spring 1986 on 35 watersheds in the SBRP, selected in conjunction with the National Stream Survey (NSS) Pilot Study. The ELS and NSS are both part of the NSWS. The third soil survey was conducted on 36 stream watersheds in 1987 and 1988. The three soil surveys included:

1. mapping watershed soils;
2. mapping vegetation;
3. mapping estimated depth to bedrock in the watersheds;
4. mapping bedrock geology from existing geology maps; and
5. sampling soils for analysis of physical and chemical properties.

#### 1.4.2.2 Levels of Analysis

The response of watersheds on a regional basis to acidic deposition was assessed using three increasingly complex levels of analysis known as Level I - Empirical Relationships, Level II - Single Factor Response Time Estimates, and Level III - Dynamic Watershed Modeling. The DDRP was an applied project, using existing techniques and models for these analyses. Each level of analysis, from Level I (least complex) to Level III (most complex), contains decision criteria that permit classification of the watershed response.

Level I analyses include statistical procedures such as cumulative frequency distributions, cluster analysis, and bivariate/multivariate regression procedures, as well as steady-state calculations such as sulfur input-output budgets, watershed indices, and equilibrium chemistry predictions. These

analyses associated available watershed attributes with surface water characteristics to define ranges of parameters that appear to affect the surface water response to acidic deposition. The Level I analyses are discussed further in Chapter 4, Empirical Relationships and Aggregation.

The Level II analyses represented single process (sulfate adsorption, cation exchange) time estimates for the rate of change and time to criterion values of specific chemical constituents, such as soil-solution sulfate and base cation concentrations (e.g., time to sulfate steady state, time to zero ANC). Because the models used for these estimates considered the dynamics of only a single process, the results were intended principally as bounding estimates of rates of change. These single factor response time estimators were used to estimate the rate of change of individual factors believed to exert significant control on surface water acidification, such as sulfate adsorption and base cation supply. Base cation supply includes weathering and/or ion exchange. These analyses are discussed further in Chapter 5, Aggregation for Base Cation Analyses, and Chapter 6, Aggregation for Sulfate Adsorption Analyses.

In the Level III analyses, integrated, process-oriented watershed models were used to project long-term changes (i.e., 0 to 50+ years) in surface water chemistry as a function of current and alternative levels of acidic deposition. The models used in this analysis integrate current understanding of how various processes and mechanisms interact and respond to acidic deposition. These mechanisms included soil-water interactions (including soil water contact time), sulfate retention, base cation exchange and replacement of base cations through mineral weathering, and other watershed processes (e.g., vegetative uptake, in-lake processes, organic interactions). The projected changes in surface water chemistry over time were used with the results from the other levels of analysis to categorize the watershed responses and estimate the number and geographic distribution of watersheds in each response category. The Level II and Level III analyses were conducted and evaluated under both current and alternative levels of acidic deposition. The Level III analyses are discussed in Chapter 7, Aggregation for Dynamic Watershed Modeling.

## 1.5 AGGREGATION PLAN ORGANIZATION

The Aggregation Plan describes the proposed approaches for aggregating the physical and chemical data from the DDRP soil survey. The Plan is organized as:

- Introductory Chapters
  - DDRP Soil Survey Design (Chapter 2)
  - Rationale for Aggregation (Chapter 3)

- Analyses
  - Empirical Relations and Aggregation (Chapter 4)
  - Aggregation for Base Cation Analyses (Chapter 5)
  - Aggregation for Sulfate Adsorption Analyses (Chapter 6)
  - Aggregation for Dynamic Watershed Modeling (Chapter 7)
- Aggregation and DDRP

## SECTION 2
## DESIGN OF THE DIRECT/DELAYED RESPONSE PROJECT

### 2.1 BACKGROUND

The DDRP was initiated to study the relationship between watershed properties (chemical and physical) and surface water chemistry and to make regional projections of future surface water chemistry as a function of current or varying levels of acidic deposition. The data for the DDRP were obtained from 145 lake watersheds in the NE, 36 stream watersheds in the M-APP, and 35 stream watersheds in the SBRP. The northeastern DDRP watersheds are a subsample from the NSWS Eastern Lake Survey (ELS). The SBRP stream watersheds are a subset of the streams surveyed by the pilot survey of the NSWS National Stream Survey (NSS) and the M-APP stream watersheds are a subset from Region 2CN, 2BN, and 1D of the NSS.

The procedures for selecting the DDRP sample differed somewhat among the NE, M-APP and the SBRP, primarily because of the differences in the ELS and NSS Pilot Survey sampling designs. Some background on the design of these two surveys is provided here because of their influence on the DDRP analyses. Complete details are provided by Linthurst et al. (1986), Messer et al. (1986), and Kaufmann et al. (1988).

### 2.2 ELS DESIGN

#### 2.2.1 Phase I of the ELS

Phase I of the ELS (ELS-I), conducted in the fall of 1984, sampled over 1,600 lakes in the eastern United States The ELS sampling approach was to use a stratified design with population-based sampling in each sampling stratum. The major geographic regions in the Survey (i.e., Northeast, Upper Midwest, Southeast) were divided into subregions based on physiographic features. Each subregion was further divided into three mapped strata based on the surface water ANC expected to dominate in different areas. The surface water ANC expected or projected in each stratum was based on a national map of surface water alkalinity that indicated areas with low alkalinity and, therefore, areas potentially susceptible to acidic deposition (Omernik and Powers 1983). Stratum 1 was chosen as projected ANC $< 100\ \mu eq/L$, stratum 2 as $100 <$ projected ANC $< 200\ \mu eq/L$, and stratum 3 as projected ANC $> 200\ \mu eq/L$. A probability sample of about 50 lakes in each stratum was selected from a list of all lakes delineated on 1:250,000-scale USGS maps, using systematic sampling with a random start. Some of the sample lakes were subsequently classified as nontarget lakes and dropped from the sample. These nontarget lakes, for example, might have turned out to be wetlands, rivers, or other systems at the time of sampling reconnaissance. Because the strata in the ELS included different numbers of target population lakes, the above design resulted in varying inclusion probabilities among strata. (The inclusion probability for a lake in the target population is the

probability of its being selected for sampling.) This has important implications for data analysis and DDRP subsample selection.

### 2.2.2 DDRP and ELS Phase II Lake Selection

At the time the DDRP subsample of lakes was selected, the lakes for the seasonal sampling phase of the ELS (Phase II) were also being chosen. Preliminary data from ELS-I (the synoptic survey) were used to identify lakes of low interest, such as high alkalinity (ANC > 400 $\mu$eq/L) lakes, shallow lakes (< 1.5 m deep), or anthropogenically disturbed lakes. These lakes were excluded from consideration as DDRP or ELS Phase II (ELS-II) lakes. Very large lakes (surface area > 2000 ha) were placed in a reserved category and also excluded from sampling for the present ELS-II or DDRP. Large lakes exhibit considerable spatial variability in chemistry and fish populations that would be difficult to characterize seasonally. Because these lakes represented less than one percent of the ELS-I target population, the large expenditure of funds that would be required to adequately characterize this resource was not warranted and large lakes were excluded. A concurrent constraint on lake selection for both DDRP and ELS-II was that for any subset of lakes, a sample size of about 50 per group was required to maintain required statistical precision. Logistical considerations for both the DDRP and the ELS-II samples limited the number of lakes and watersheds that could be adequately characterized to about 150. In order to satisfy these constraints, the ELS-I sample was split into three groups using cluster analysis on the ELS-I data. After examination of the clusters produced by means of over 30 variables describing the physical and chemical status of the lakes, the lakes were split into groups based only on ANC. ANC was used because (1) it was a primary criterion variable in separating the cluster of acidic and very low ANC lakes from the other clusters, (2) it indicated the current lake status, and (3) it integrated base cations, with mineral and organic acidity to indicate potential susceptibility to acidic deposition. The three groups were defined as (1) ANC < 25 $\mu$eq/L, (2) ANC 25-100 $\mu$eq/L, and (3) ANC 100-400 $\mu$eq/L.

The DDRP and ELS-II both required a sample size of about 50 lakes per cluster. The DDRP had a constraint, however, not present for the selection of ELS-II lakes. Watersheds with areas greater than 3,000 ha could not be adequately mapped during the soil survey phase of the DDRP. To accommodate this constraint, 60 lakes were selected from each of the 3 ANC groups using a systematic variable probability sampling scheme that resulted in approximately equal inclusion probabilities within clusters. After the sample was selected, lakes with watersheds too large to be readily mapped were dropped from the DDRP sample. The sample of 60 was randomly reduced to 50 for the ELS-II sample. Thus, DDRP and ELS-II lakes overlap by about 85%.

Several lakes were dropped from the sample because access was denied. This resulted in a total DDRP sample size of 145 lakes: 49 in ANC Group 1 (< 25 $\mu$eq/L), 49 in ANC Group 2 (25-100 $\mu$eq/L), and 47 in ANC Group 3 (100-400 $\mu$eq/L).

### 2.3 NATIONAL STREAM SURVEY DESIGN

The NSS began in 1985 with a Pilot Survey in the SBRP. The Pilot was conducted to establish the methodology for carrying out a broad regional survey of streams. The Pilot Stream Survey framed the target population by defining a stream reach as the length of 'blue-line' stream on USGS 1:250,000-scale maps that lies between the downstream and upstream confluences with other blue-line streams, or the upper boundary if no upper confluence is present.

A two-stage sampling approach was designed for selecting NSS streams. In the first stage, the a point frame was used to select the sample of stream reaches. A rectangular grid of points, separated by a scaled distance of approximately 13 km (8 mi), was positioned at random over a 1:250,000-scale topographic map. The first stream reach intersected by a line from each point drawn downslope perpendicular to the contour lines was included in the first stage sample. If any portion of the reach extended outside the study region, if the reach drained directly into a reservoir, or if a watershed was too large [> 150 km$^2$ (60 mi$^2$)], the reach was designated non-interest and dropped from the sample.

The first stage sample was used to establish the physical characteristics of the stream reach population, e.g., the distribution of reach lengths and drainage areas. A second stage sample was selected for chemical sampling by designating reaches corresponding to every other grid point. Fifty-one stream reaches were sampled for water chemistry in the Pilot Stream Survey.

### 2.4 DDRP SOIL SURVEY DESIGN

Once the sample of watersheds to be characterized had been selected, the soil surveys proceeded in a similar manner in the NE, the M-APP, and the SBRP. Because the DDRP had a regional focus, the results of the soil survey had to be extendable to the target population of systems. Each soil survey was designed so that any attribute that could be defined for a watershed could be extrapolated to the respective target population attribute through the probability structure of the sample. The DDRP faced a major difficulty with the design. The aim of the project was to characterize the soil chemistry of the sample watersheds. However, we do not "measure" the soil chemistry of a watershed. At best, we can excavate a soil pit (or several pits), describe and sample the soil from the pit, and chemically characterize the soil samples. The measured results represent the chemistry of the soil from that pit, and, to some extent, represent the chemistry of adjacent soil. We know, however, that soil chemistry shows significant spatial variability over the extent of a

watershed so that the soil taken from a single sampling site (pedon) on a watershed, does not necessarily represent soils over the entire watershed and the entire region of concern.

### 2.4.1 Watershed Mapping

In order to surmount this difficulty, the DDRP drew on the experience and knowledge of soil spatial characterization in the U.S. Soil Conservation Service (SCS). The SCS specializes in mapping the distribution of soil types within watersheds. Arrangements were made with the SCS to map all 217 DDRP watersheds and prepare maps of soil, vegetation type, estimated depth to bedrock, bedrock geology, and land use. Soil scientists defined and delineated segments of the landscape with similar kinds and extent of soils, called map units. The map units was either soil consociations or complexes. The extent of major map unit components and minor components (inclusions) were estimated to the nearest five percent. The soil mapping consisted of delineating each occurrence of a map unit on a watershed, with a lower limit of resolution of 2.4 ha (6 ac). Map units were regionally correlated and defined. A soil map was prepared for each watershed, showing the outline of each map unit on the watershed. The maps and map unit delineations were digitized for entry into a computerized geographic information system (GIS). The area in each map unit polygon delineated on each watershed was calculated by the GIS, and the area and percent of watershed area in each map unit were tabulated by watershed. The composition of each map unit was also entered into a computer database. By merging the two data files, researchers could calculate the area and percent of each kind of soil or miscellaneous area by watershed.

### 2.4.2 Sample Class Delineation

The ideal way to characterize the soils of a watershed would be to take several samples from each kind of soil. For a regional survey, such as the DDRP, this approach was unrealistic. It is not cost effective, and for the DDRP in particular, it also was not feasible. For example, approximately 600 soils were identified in the 145 NE watersheds. Human resources and time constraints limited the total number of soil pedons that could be sampled in the NE to around 300. Similar situations existed in the M-APP and the SBRP, although on smaller scales.

To increase the efficiency of soil sampling, soil components (e.g., soil series) were grouped into classes believed to have similar chemical and physical properties. The primary consideration in grouping soil components was the expected interaction of the soils with acidic deposition. For NE soils, groupings were determined at a week-long workshop attended by northeastern soil scientists. The results of this process have been published by Lee et al. (1989b). A combination of published information and experience with northeastern soils were used to define 38 groups of similar soils or soil sampling classes. The result of the workshop was that similar soil components were placed into these sampling classes. Similar workshops were held for the other two regions following the mapping

place of each soil survey. Twelve sampling classes were defined for the SBRP and 15 were defined for the M-APP. The sampling classes delineated for the NE, SBRP, and M-APP are shown schematically in Figures 2-1, 2-2, and 2-3, respectively.

Every regionally identified soil component was assigned to a sampling class. An assumption of the sampling structure was that the soil components within a sampling class were enough alike for any sample from the class to be used to characterize that class. Operationally, this means that the aggregate properties of the sampling class are assigned to every member of the class. An estimate of the distribution of sampling classes on each watershed was obtained through the mapping. It follows that soil chemical and physical properties can be associated with every point in the watershed. This permits computation of an aggregate value at the watershed scale for any variable that was measured or calculated at the pedon level. Inasmuch as that variable, and others, can be defined at the watershed level, regional descriptions of the variable (e.g., averages or distributions) can be obtained through the sample probability structure.

## 2.5 AGGREGATION

The chemistry of any lake or stream represents the integrated response of its entire watershed. Deposition loadings, hydrologic flow paths, types of soils, vegetation cover, bedrock geology, and physiographic features of the watershed all affect water chemistry. Arriving at watershed level estimates of soil chemical and physical data requires the combination of soils data collected at specific points. The goal of any aggregation procedure is to describe the functional integration that corresponds to the operational integration occurring in the watershed. The obvious approach is to define watershed level quantities as a weighted combination of the soil sampling classes that occur on the watershed. There are several possibilities that can reasonably be considered as weights. One weighting scheme is simply the percentage composition of the watershed in terms of the sampling classes (i.e., each sampling class receives as its weight its areal percentage on the watershed). This, however, may not be the average that functionally integrates watershed characteristics with the appropriate surface water chemistry response. The sampling class quantities could also be weighted, for example, by soil depth, proximity to a lake or stream boundary, vegetative cover type, or bedrock geology. In fact, the weight function might depend on the variable being studied, so that sulfate

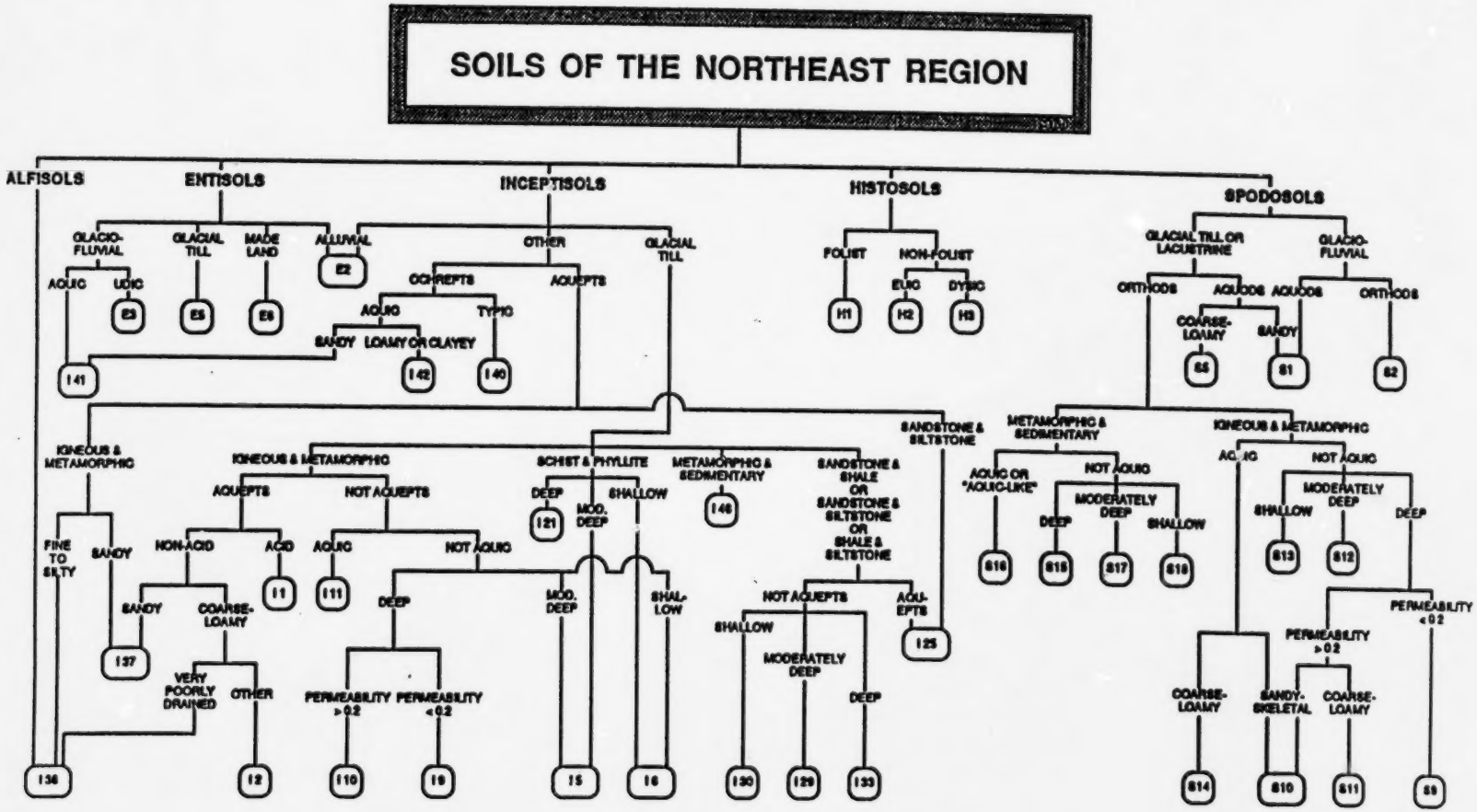


Figure 2-1. Soil sampling classes for the Northeast.

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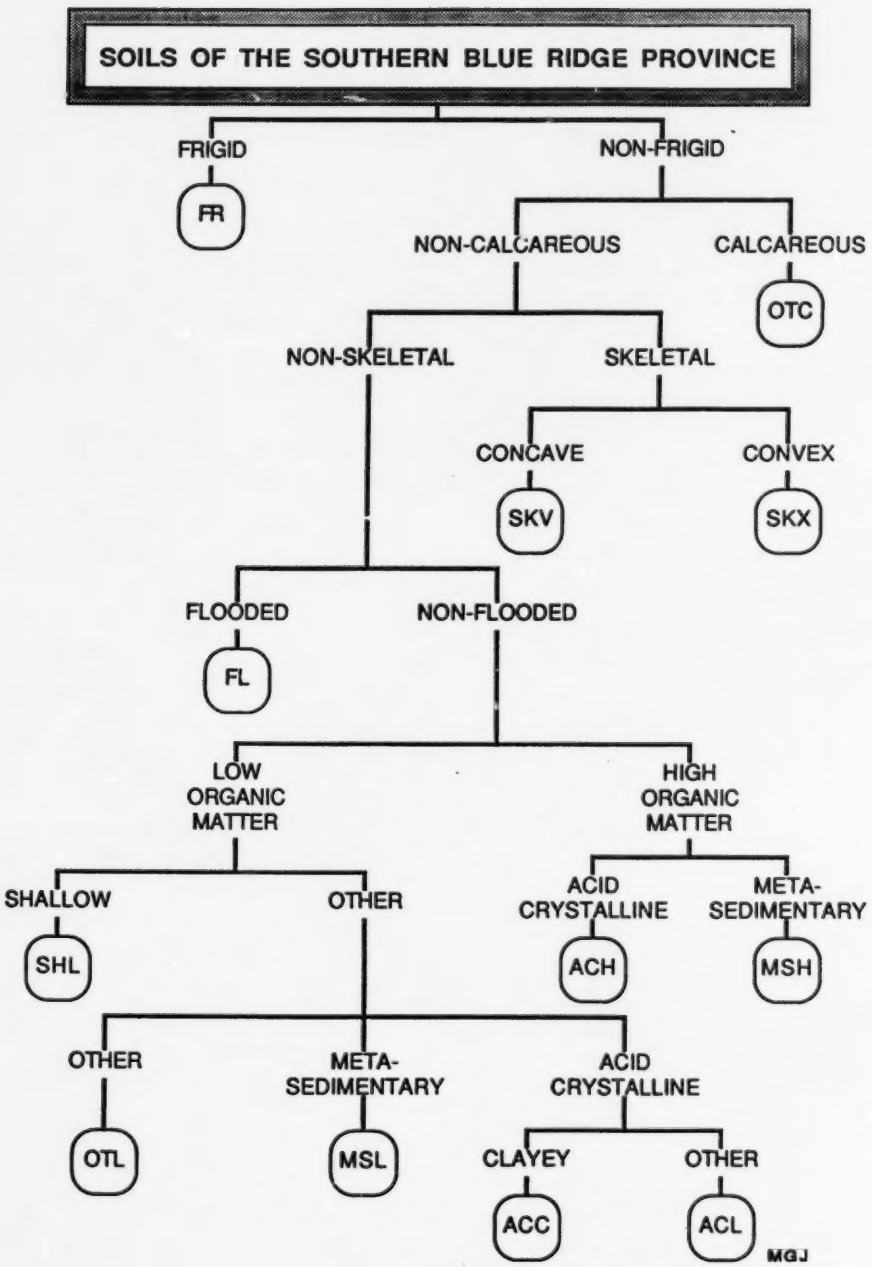


Figure 2-2. Soil sampling classes for the Southern Blue Ridge Province.

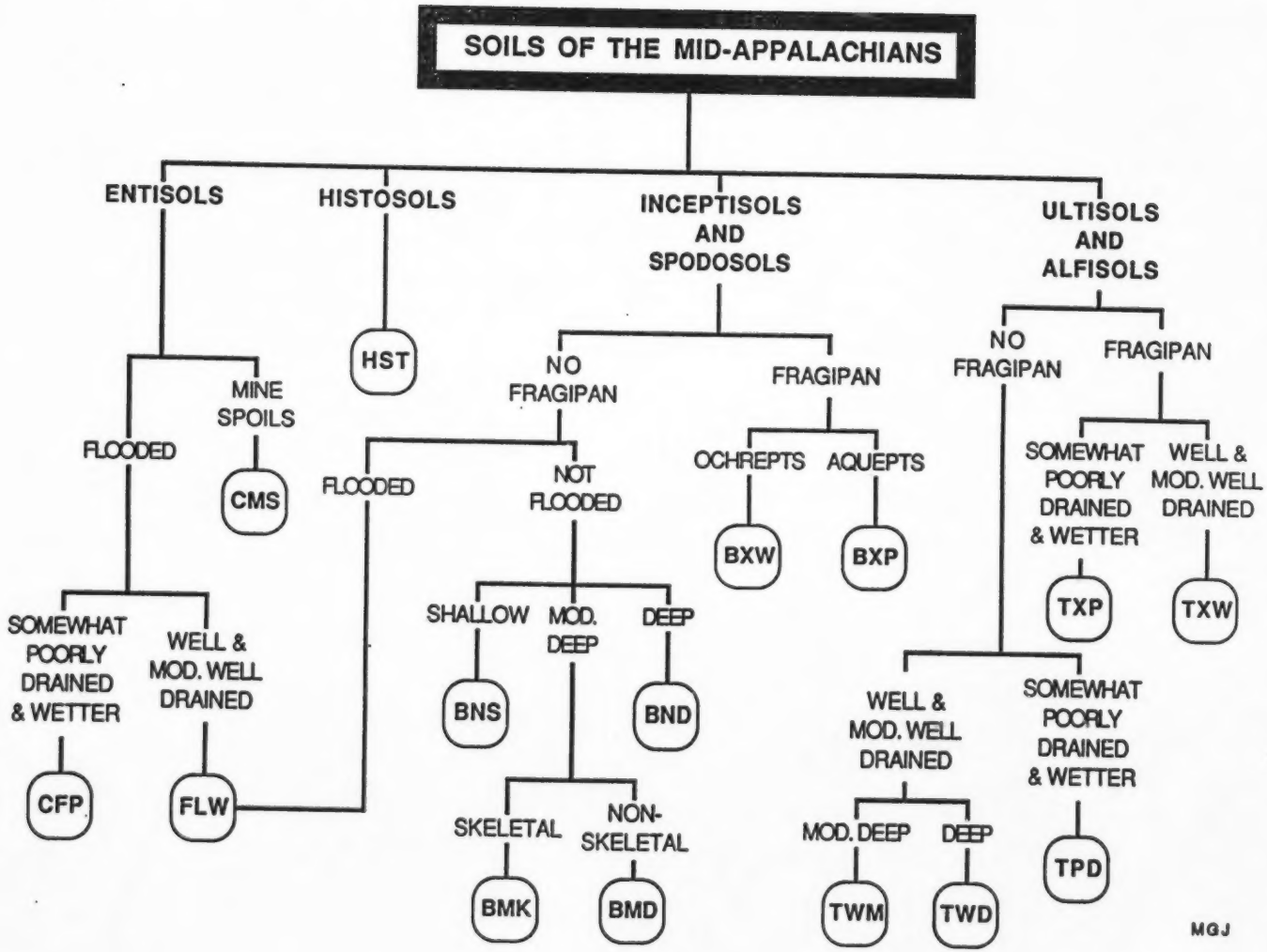


Figure 2-3. Soil sampling classes for the Mid-Appalachians.

adsorption would not necessarily be aggregated in the same manner as base cations. In all likelihood, capacity and intensity variables should have different aggregation algorithms.

Central questions related to data aggregation include:

- How should pedon information be aggregated to the sample class?
- When and to what extent should the pedon data be aggregated?;
- Should pedons be integrated vertically?;
- Should the integrity of soil horizons be maintained up to the watershed level (Figure 2-4).

The aggregation approach selected should reflect the physical and chemical attributes of the watershed. This aggregation plan describes and evaluates the specific approaches used to develop and select among several aggregation techniques for each of the DDRP Levels of Analysis.

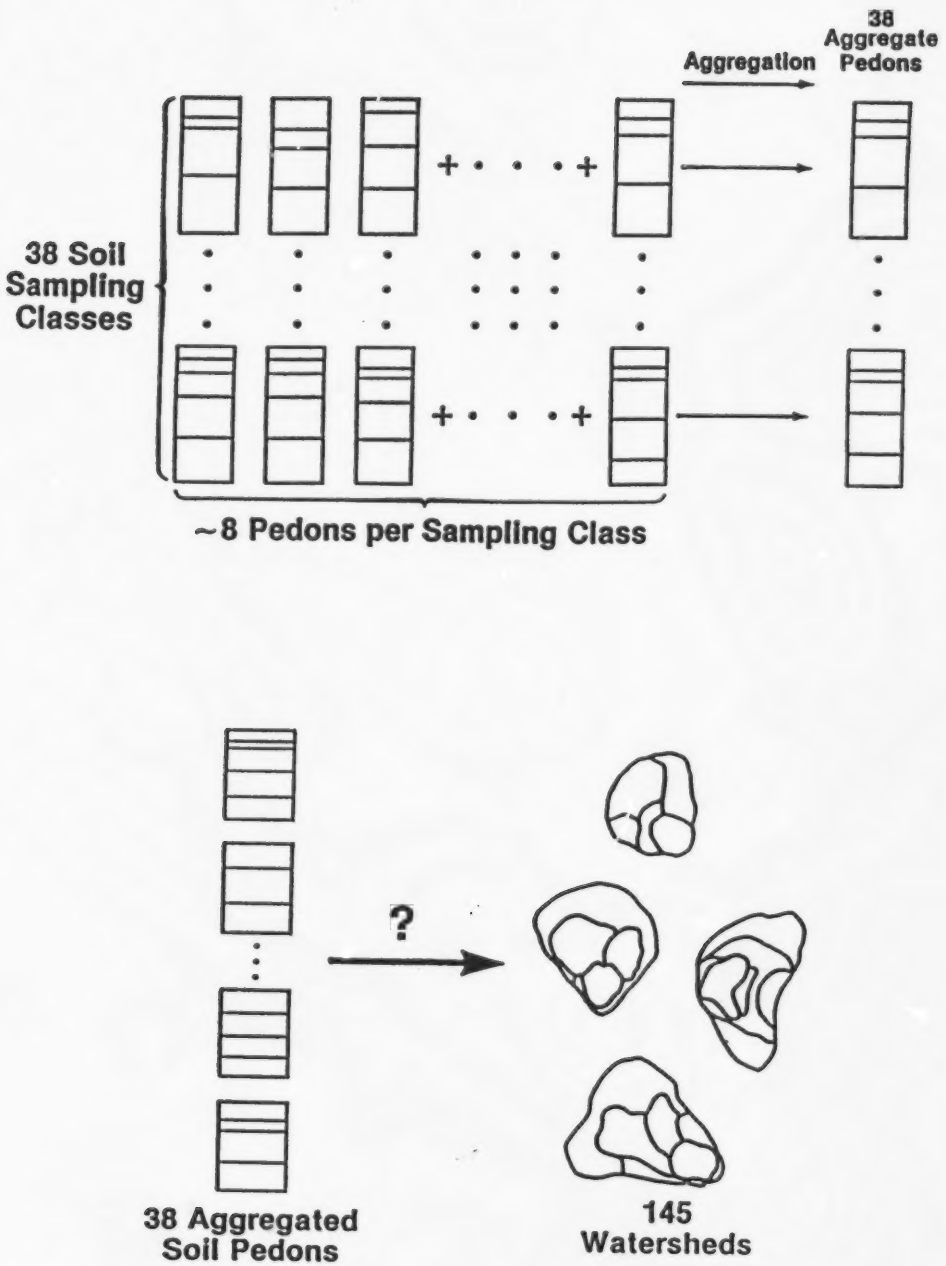


Figure 2-4. Example of the aggregation problem for soils within a watershed.

# SECTION 3
# RATIONALE FOR AGGREGATION

## 3.1 INTRODUCTION

Ecosystems are complex, with the system response to a perturbation reflecting the interaction of the abiotic and biotic system components. Forcing functions, or external inputs and internal processes, important in the functioning of ecosystems, generally occur over several orders of magnitude in both space and time. Aggregation or averaging of these processes and functions in space and time, therefore, represents a generic problem in systems analysis. The aggregation issue, in fact, represents part of two major problems in ecosystem ecology. These two problems are:

1. identifying and measuring the forces and processes that operate over more than one scale; and
2. developing general procedures for aggregating data, processes, and process interactions occurring at different scales [Risser 1986, Rosswall and Woodmansee (in press)].

Procedures generally are available for identifying and describing spatial and temporal variability in soils, vegetative cover, species diversity and abundance, or other watershed attributes. The inverse issues of aggregating sets of heterogeneous data and the formulation of specific procedures for aggregation, however, have received surprisingly little attention.

## 3.2 PREVIOUS STUDIES

Previous regional analyses of relationships between watershed characteristics and surface water chemistry in areas with varying levels of acidic deposition have generally been data limited, so aggregation within watersheds was not an issue (e.g., Rapp et al. 1985, Nair 1984, Eilers et al. 1983). Hunsaker et al. (1986), however, used more intensive soils data and maps in the Adirondack Data Base and found that different aggregation procedures resulted in different correspondences or associations between soil characteristics and surface water chemistry. The aggregation approaches that incorporated considerations of soil hydrologic groups as one of the factors usually had the best associations (as defined by $R^2$ values) with surface water chemistry.

Theoretical studies of the influence of aggregation on mathematical model simulation uncertainty have been conducted by several authors. O'Neill and Rust (1979) evaluated the effect of potential aggregation error or uncertainty in a theoretical ecological model and provided several simple rules for minimizing aggregation error, including lumping components with similar turnover times and lumping rare species with common species. Gardner et al. (1982) expanded on this earlier study and conducted a robust analysis of aggregation error in 40 linear and nonlinear models. This

study indicated that no errors were introduced through aggregation when the two components had identical turnover times. Gardner et al. (1982) also concluded that the aggregation error was less than 10% if the components (i.e., respiration, mortality) were not linked in series, and the loss rates differed by less than a factor of three. Although there are some practical rules for aggregation, the aggregation dilemma is far from resolved (Gardner et al. 1982).

The aggregation issue also has received some attention for applied problems. Wosten et al. (1985) described a procedure for aggregating soil horizons from a watershed survey into representative mapping units for use in a regional soil water simulation model. A detailed soil survey was used to obtain soil physical data for a model of the water regime in the unsaturated zone. Nine major soil horizons were defined for the survey area in terms of texture, structure, organic matter content, and bulk density (Wosten et al. 1985). Hydraulic conductivity and moisture retention curves were made in each major horizon to develop average curves. Statistical comparisons among these curves and the major soil horizons indicated that only five major horizons were required to characterize the survey area. Data from these five horizons were than transformed to obtain characteristic sequences of these horizons that were used in the modeling exercises. Using this aggregated data in the simulation model resulted in excellent agreement between calculated and measured evapotranspiration for three years (Wosten et al. 1985). Additional studies using similar approaches, however, are extremely limited.

There currently are no universally accepted or generalized procedures for aggregating watershed components to obtain a watershed weighted average or characteristic value. This is not surprising because both aggregation procedures and subsequent analytical techniques (e.g., statistical analyses, mathematical models, etc.) are developed to address specific objectives and are applied to specific, often very limited, data sets. A variety of aggregation procedures could have been used to satisfy the objectives of the various DDRP levels of analysis.

### 3.3 AGGREGATION APPROACHES

A number of approaches could have been used to obtain an aggregated watershed estimate for any watershed attribute (Figure 3-1). These estimates range from simple arithmetic or mass-weighted average values (Figure 3-1) to weighting by hydrologic group (e.g., SCS hydrologic classification or permeability estimates), bedrock type [e.g., Norton's bedrock classification (Norton 1980)], vegetation type (e.g., open, mixed coniferous vs. deciduous), or other characteristic to obtain a weighted watershed estimate. Aggregation procedures do not necessarily have to precede analyses (Figure 3-2). Associations between individual soil pedon horizon parameters and surface water chemistry can be investigated prior to data aggregation. Analyses can be conducted on individual

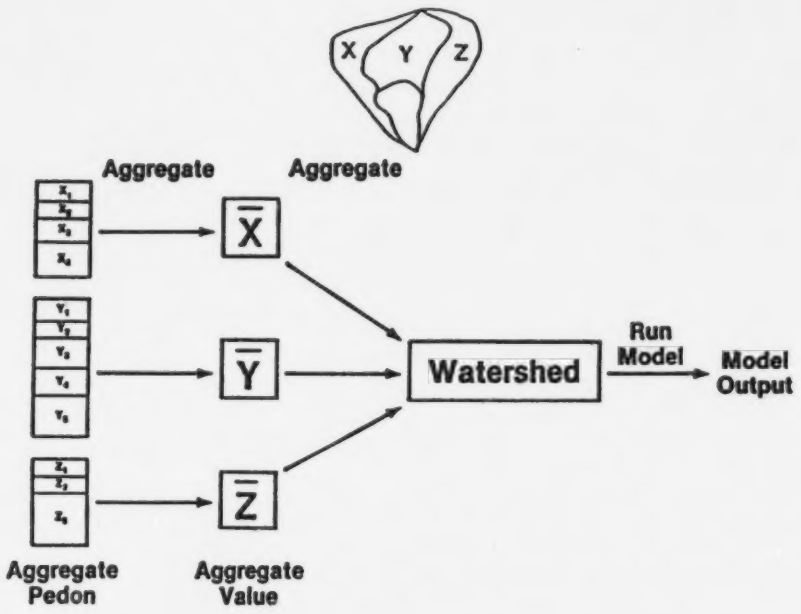


Figure 3-1. Aggregation of watershed soils before model application.

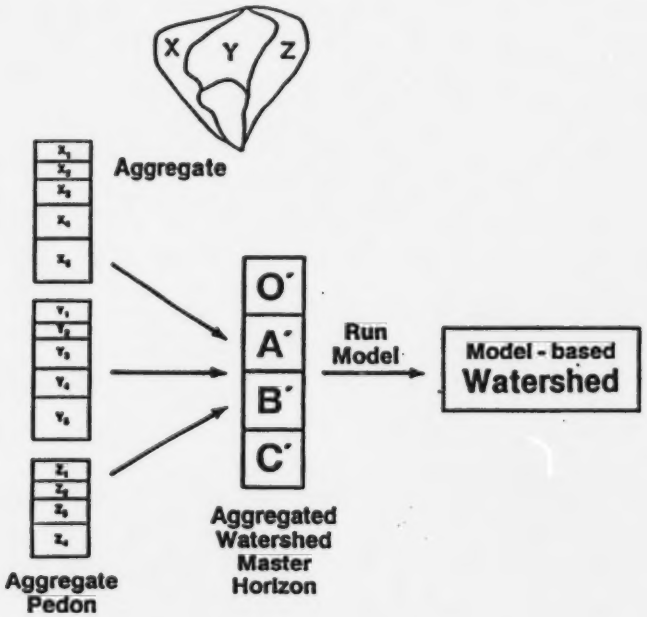


Figure 3-2. Aggregation of watershed soils to master horizons followed by model application and subsequent aggregation for watershed response.

pedon soil horizons, with the model forecasts subsequently aggregated or averaged to obtain an estimated watershed response to acidic deposition.

Many aggregation procedures could have been used with the soils data or analytical results to estimate the expected watershed response to acidic deposition. We initially identified more than 35 possible aggregation approaches. Based on first principles, our current understanding of watershed processes, and the observed aquatic system response to acidic deposition, we selected a small number of these aggregation approaches for consideration and use in the DDRP.

### 3.3.1 Generic Approaches

The aggregation procedures discussed here were selected from many possible approaches in a multi-level process that began with a rigorous screening based on physical principles. Although some aggregation schemes are specific to the level of analysis (e.g., correspond to explicit model formulations of watershed processes), there were two generic considerations for each of the aggregation approaches: hydrologic flow path and hydrologic contributing watershed area.

#### 3.3.1.1 Hydrologic Flow Path

The surface water response reflects the interaction and processing of acidic deposition by the watershed soils. This interaction occurs as water flows through the soil past soil exchange sites where sulfate is adsorbed, hydrogen ions are exchanged for base cations or aluminum, and other processes such as reduction, uptake, or decomposition occur in the soil matrix. If water does not move through a particular horizon, these exchanges will not occur and that horizon will not influence the surface water chemistry. Including such horizons in the aggregated data for the watershed is unwarranted because the attributes of that horizon are not contributing to the surface water response. Factors such as SCS hydrologic group or horizon permeability may be useful surrogates for indicating potential hydrologic flow paths and differentially weighting horizons during aggregation. For example, weighting classes by SCS hydrologic group was considered because such weighting could provide a surrogate for explicitly modeling hydrologic pathways. The SCS classifies soil types by hydrologic groups ranging from A to D. Definitions of these hydrologic groups are based on the infiltration rate of water entering the soil at the surface, which is related to the runoff potential. Soils classified as hydrologic group A have high infiltration rates and low surface runoff potentials. Soil-water contact, therefore, would probably be higher than in soils with low infiltration rates. Soils range along a continuum of runoff potential from A to D, where soils classified as hydrologic group D have low infiltration rates and high surface runoff potential.

Hydrologic group represents one estimate of potential flow path, but this grouping is based principally on surface properties (infiltration, runoff) and not necessarily on flow properties within the

soil. An estimate of permeability or percolation through the soil horizon was likely to be a better surrogate for flow path. In this approach permeability for each horizon was estimated based on the horizon texture class (Brakensiek et al. 1981) or obtained from the National Soils Handbook (Soil Survey Staff, 1983) and used to weight horizons for aggregation.

#### 3.3.1.2 Hydrologic Contributing Watershed Area

By definition, a watershed contributes to surface water quantity and quality. The entire watershed area, however, may not contribute uniformly to stream flow and surface water quality because of differential contributing areas of hydrologic flow paths. In the DDRP analyses, buffer strips of 10, 30, and 100 meters adjacent to the lake or stream, and along contributing water courses in the watershed, were delineated. Physical and chemical characteristics of the soils in these zones are likely to have a much stronger relationship with stream chemistry than inclusion of all the watershed soils, because they are the last point of hydrologic contact. These contributing areas can be used to differentiate weight horizons during the aggregation procedure. The contributing watershed area can be used independently or combined with surrogates of hydrologic weight to obtain a combined weight for aggregating soils to the watershed level.

The SCS hydrologic group may serve as a surrogate for both water flow path and contributing watershed area (i.e., landscape position). The hydrologic designation, indicates the potential for surface or near-surface runoff and ranges from highly permeable soils with low runoff potential (Group A) to highly impermeable soils with high runoff potential (Group D). Hydrologic groups also appear to be correlated with the geomorphic position on the watershed. This designation, therefore, may indicate soils located near intermittent or permanent water courses and, therefore, soils that have the last contact with water before it enters the receiving surface waters. The weights associated with each hydrologic group currently are being evaluated with a portion of the soil survey data.

#### 3.3.1.3 Generic Analytical Approach

Many of the analyses described in subsequent chapters have outputs that are tied to a measured water chemistry property such as ANC or sulfate concentration. The evaluation of aggregation approaches considers only linear relationships between watershed attributes such as percent base saturation or soil solution sulfate concentration (which may be the output of a nonlinear, dynamic model) and water chemistry (e.g., Ca or $SO_4$ concentration). Monotonic relationships, even if nonlinear at some level of resolution, still permit the detection of linear trends. We can use the measure of linear trend as a goodness of fit criterion to guide the selection of an aggregation scheme. The $R^2$ statistic from multiple regression measures the correlation of a response with the explanatory variables; that is, it measures the strength of the linear relationship between the response (e.g., lake ANC concentration) and the explanatory variables (e.g., soil percent base saturation or hydrologic

group). Although it is possible to find more sophisticated statistics, $R^2$ is an eminently suitable screening criterion.

The $R^2$ statistic, however, is not an absolute rule. Other criteria include, for example, the simplicity and scope of an aggregation method. Of two methods with nearly equal $R^2$ values, the simpler method is preferred over the more complex method. Also, a method that gives a high $R^2$ for several soil-water chemistry parameter pairs is given preference, even though it may not provide the maximum $R^2$ for any individual analysis. This process should be tempered by scientific judgment as to which analyses are more important for characterizing these relations.

### 3.3.2 Common Approach

Although there are many possible aggregation approaches, extensive discussions among the DDRP investigators resulted in the formulation of one aggregation approach that was applied to each level of analysis. For capacity variables (e.g., cation exchange capacity, sulfate adsorption capacity), the common aggregation is as follows:

1. Weight each subhorizon by its mass [thickness * bulk density * (1- percent coarse fragments)] to obtain a mass-weighted average Master Horizon (O, A, E, B, C) value for each pedon.
2. Use the Arithmetic average of within-sample-class master horizons to obtain weighted sample class master horizon values.
3. Weight the master horizon value by the areal proportion of the sampling class on the watershed to obtain a watershed-weighted average estimate for each master horizon.
4. If desired, weight the value for each master horizon by thickness or mass to obtain a single watershed weighted average value. (The need to include this step was model specific, because some models required a single watershed parameter value while others used the individual soil master horizon parameters.)

In the DDRP soil surveys, each distinct subhorizon greater than 3 cm thick in the sample pedons was sampled. Although subhorizons can be recognized in the soil profile, the most prominent horizons are the master or major horizons such as O, A, E, B, and C. Each of the master horizons is distinguished pedologically based on various soil properties and processes (National Soils Handbook 1983). The O and A master horizons are distinguished primarily by the amount and state of the organic matter present. The O master horizon is distinguished by the surface accumulation of organic matter overlying mineral soil. The O master horizon is subdivided into subhorizons based on the degree of decomposition of this organic matter. The A master horizon is identified by the accumulation of humified organic matter mixed with mineral fractions, the latter fraction being dominant. The other master horizons are similarly identified (National Soils Handbook 1983). The

master horizons reflect different soil forming processes. The effects of these processes determine the particular horizon attributes such as sulfate adsorption capacity, exchange capacity, and other characteristics influencing surface water chemistry. Combining the subhorizons to the master horizon, then, represents the first logical step in aggregation. Bulk density adjustments are critical for capacity variables because these variables represent the pool of soil material potentially available to react with acidic deposition.

Changes in the soil pH of the horizons depend on the capacity variables associated with them, such as cation exchange capacity and amounts of weatherable minerals. These capacities are directly related to the mass of the horizons; given equal amounts of acidic deposition and equal soil characteristics for each horizon, a 10-cm thick horizon would change more quickly than a 30-cm horizon. In contrast to the importance of soil mass for weighting capacity variables, the effects of intensity variables on water chemistry do not depend on the volume or mass of soil having those characteristics. For example, water flowing from a 10-cm thick horizon with a soil pH of 5.0 would have the same pH as water flowing from a 30-cm thick horizon with a soil pH of 5.0.

For intensity variables (e.g., % base saturation or equilibrium soil sulfate concentration), the following approach was used:

1. Using the average (arithmetic) subhorizon chemistry within each major horizon of individual pedons to obtain a master horizon average chemistry, weighting the lowest horizon in each group more heavily; if there were more than two subhorizons per horizon, the upper subhorizons were averaged and this average value further averaged with the lowest subhorizon in the horizon. If there were only two subhorizons per horizon, the value in the lowest subhorizon was doubled before averaging.
2. Average (arithmetic) the master horizon chemistry across pedons within a sampling class.
3. Weight master horizons by the area of the sampling class on the watershed to obtain average values by master horizon for the watershed.
4. Average the horizons data for master horizons, weighted by thickness, to obtain an average watershed value.

Intensity variables are measured as concentrations and reflect the last soil horizon(s) with which the water comes in contact. The lowest horizons, therefore, were weighted more heavily. In the Level I analyses, the master horizon designations were used as explanatory variables in the statistical/exploratory analyses. The Level II and III analyses also used the master horizon as the operational unit. The following sections, evaluate these aggregation approaches, along with other

possible aggregation schemes. The objective was to use a common approach for all levels of analysis and for all soil/surface water variables.

### 3.3.3 Aggregation Evaluation

Subsequent chapters discuss the specific application of aggregation schemes within the DDRP Levels I, II, and III analyses and the approaches used to evaluate these aggregation procedure alternatives. The general format for each chapter is:

1. Problem Statement
2. Background/general theory for this level and previous aggregation approaches, (if any)
3. Specific Aggregation Approaches
4. Evaluation of Aggregation Schemes

# SECTION 4
# EMPIRICAL RELATIONSHIPS AND AGGREGATION

## 4.1 PROBLEM STATEMENT

The specific objective of the DDRP Level I analyses was to statistically correlate the numerous climatic, geologic, physiographic, hydrologic, soils, vegetation, and land use data collated in the DDRP data base with the surface water chemistry in the DDRP watersheds. Bivariate and multivariate analyses of several types were used to perform these tests and satisfy the DDRP objectives.

For each of these analyses, a statistical mean was needed to reduce the data collected for each watershed to a single calculated or index value for the parameter in each watershed. This may be as simple as determining the percentage of conifer vegetation type on a watershed or as complex as determining a representative base saturation for a watershed by weighting data for individual soil horizons and spatially distributed soil sampling classes according to how much water flows through each horizon or the proximity of that sampling class to surface water. The remainder of this section discusses how this data aggregation was accomplished and evaluated for the DDRP Level I analyses.

## 4.2 BACKGROUND

### 4.2.1 Previous Data Aggregation Approaches

Previous regional analyses of empirical relationships between watershed characteristics and surface water quality variables have generally been so data limited that aggregation within watersheds was not an issue (e.g., Rapp et al. 1985; Schnoor et al. 1986; Nair 1984; Eilers et al. 1983). Hunsaker et al. (1986) found that vertically averaging soil horizons, weighting according to hydrologic group, and then horizontally averaging across watersheds, weighting according to the areal percentage of each soil type, gave the highest correspondence (i.e., highest $R^2$) between soil characteristics and surface water chemistry. They did not have data on the proximity of soils to surface water.

Modeling solute transport through soils (e.g., for agricultural operations or waste disposal) is an area of active study and research. Generally, such models use empirical measurements and scaling theory or stochastic treatment of transport parameters to account for spatial variability (e.g., see review by Van Genuchten and Jury 1987). Such models, however, are not usually oriented toward predicting the chemistry of streams or lakes.

### 4.2.2 Data Aggregation Issues for Modeling Empirical Relationships

The data required for the Level I empirical analyses needed to be effective, or composite, numbers that integrate short-term and long-term hydrologic and biogeochemical processes for whole watersheds. The simplest multivariate models relate single composite values for independent variables, such as annual deposition and runoff, percent rock outcrop, soil depth, texture, slope, base saturation, sulfate saturation, organic matter content, or percent coniferous forest cover for each watershed, to dependent variables, such as the measured surface water ANC or pH for each watershed. More complex models consider each of these variables by soil horizon or by sample class or area within each watershed. The number of variables that could be entered into the models, however, was constrained by the number of watersheds sampled: 145 in the NE, 37 in the M-APP, and 35 in the SBRP.

An additional issue to be considered in aggregating data for modeling empirical or dynamic relationships between watershed characteristics and surface water chemistry is the distinction between intensity variables and capacity variables (Section 3.3.2). Water chemistry at any point in time is controlled by intensity variables such as soil pH, base saturation, equilibrium soil-sulfate solution concentration, $pCO_2$, and aluminum solubility. Changes in water chemistry over time are dependent on capacity variables, such as soil cation exchange capacity, amounts of weatherable minerals present, sulfate retention capacity (percent of equilibrium with current sulfate deposition), and amount of soluble aluminum present.

The effect of intensity variables on water chemistry is dependent on the relative cross-sectional areas of the different soils through which water flows just prior to emerging as surface water. Thus, water emerging as base flow through relatively narrow bands of high-pH, riparian zone soils will generally be less acidic than water emerging during wet seasons or during storms through broad bands of relatively low-pH, side-slope or upland soils in expanded variable hydrologic source areas. During such high-flow periods, the pH of a lake or stream segment would be determined from the mixture of water flowing through the narrow lowland area, water emerging as subsurface flow from the variable hydrologic source areas, and deposition that enters the stream or lake directly without interacting with the soils.

The Level I models needed to include primarily intensity variables, with capacity variables included only to the extent that changes in these variables might take place within a year, or over several watershed flushing times. Because the magnitude of such change was believed to be small relative to the starting values for these variables, they were, in most cases, not included in the Level I analyses. Level I aggregation, however, needed to incorporate or account for the dynamic changes in the cross-sectional area through which surface water emerges over the period of a year.

## 4.3 SPECIFIC AGGREGATION APPROACHES FOR LEVEL I EMPIRICAL RELATIONSHIPS

Results from each of the aggregation procedures discussed in this section could be compared with results from the common approach discussed in Section 3.3.2 to provide information about the effects of data aggregation upon the Level I analyses.

### 4.3.1 Aggregation to Sample Class/Horizon

This aggregation approach calculates a mean value for each horizon within each sample class, weighting the value for the lowest subhorizon in the master horizon in each pedon by thickness (intensity variables) or mass [thickness * bulk density * (1 - percent coarse fragments)] (capacity variables). This could be done for:

1. Each horizon for which there were two or more samples for the given sample class.
2. Three soil compartments, an organic compartment, an A/E/B horizon compartment, and a C horizon compartment, weighting subhorizons by thickness or mass.
3. Each master horizon, weighting each subhorizon by mass (capacity variables), or by giving the lowest subhorizon most weight (intensity variables). Chemically distinct subhorizons, such as Bw or Cg, should be kept separate from the master horizon so these critical chemical characteristics are not masked by averaging with other subhorizons.

Values for sample class/horizons could be assigned coefficients based on the permeability/hydrologic group or percentage abundance in a watershed and entered as independent variables in multivariate models (within the limits of the number of dependent observations). These same sample class/horizon values could be used by the Level II and III models and the effects compared.

### 4.3.2 Aggregation to Watershed/Horizon

Watershed properties could be aggregated to the watershed/horizon level by first aggregating to sample class/horizon as in 4.3.1. Next, a mean value for each watershed/horizon would be calculated, weighting the value for each sample class/horizon according to the predominant hydrologic group or landscape position of the sample class (depending on whether sample classes turn out to be more homogeneous by hydrologic group or landscape position).

Regression analysis could be used to determine the weights. The association between hydrologic group and/or landscape position and surface water chemical constituents could be used to identify appropriate weights. The associations that account for the largest proportion of the variance in surface water chemical constituents (i.e., highest $R^2$ values) could be used to define the weights for the hydrologic groups, A through D, and/or landscape position.

The watershed/horizon values could be entered into the Level I models as independent variables.

#### 4.3.3 Aggregation to Sample Class/Horizon, Then to Watershed Level

This approach aggregates the data to the watershed/horizon as in 4.3.2. A single mean value for each watershed then would be calculated by weighting each horizon evenly.

#### 4.3.4 Aggregation to Sample Class/Pedon, Then to Watershed Level

Another aggregation procedure could be used to calculate a mean value for each sample class horizon, weighting horizon values by thickness or mass. A mean value would be calculated for each sample class, weighting horizon values using hydrologic group weights identified in a regression-type analyses. A mean value for each watershed then could be calculated using the following procedures:

1. Area weight each sample class by its percentage abundance in each watershed.
2. Area weight each sample class by its percentage abundance within an area between the lakeshore and a line 100 m from the lakeshore (i.e., 100-m buffer).
3. Area weight each sample class by its percentage abundance within a zone between the lake or stream and the contour 40 feet in elevation above the lake.
4. Area weight each sample class according to its landscape position. The following rules apply: (a) weight sample classes in low-lying landscape positions double, (b) weight sample classes in side-slope positions even, (c) weight sample classes in upland positions by one half. The area weights are used to illustrate the concept. Weights could be determined similar to those described in Section 4.3.2.

These aggregation schemes result in the loss of horizon definition early in the procedure, but may best account for the differential influence of hydrology in different horizons and landscape positions.

### 4.4 EVALUATION OF AGGREGATION SCHEMES

The aggregation schemes were evaluated using bivariate and multivariate correlations with lake water chemistry data. The most appropriate scheme was defined as the one that consistently produced the highest correlation coefficients with surface water chemical constituents. The term, "most appropriate" is from a pragmatic, not necessarily a process, standpoint. There was a possible conflict in this approach because the same techniques proposed to evaluate the aggregation approaches also were proposed to evaluate the watershed parameters most strongly associated with surface water chemistry. Each of the aggregation schemes proposed, however, appears reasonable based on first principles.

We evaluated the results of several of the schemes to determine which watershed parameters were most strongly associated with surface water chemistry, and then attempted to determine what characteristics of each scheme led to that selection. Comparing the results of each level of analysis for the different schemes also aided the interpretation of each scheme. For example, sensitivity analyses of the models might have shown that certain variables, horizons, or watershed areas critically affected the predicted results. Such findings aided in the interpretation of the aggregation scheme and in the interpretation of watershed parameters most strongly associated with surface water chemistry. Such findings also led to reformulation of the aggregation schemes used.

## SECTION 5
## AGGREGATION FOR BASE CATION ANALYSES

### 5.1 PROBLEM STATEMENT

The purpose of the Level II base cation analyses was to make model-based forecasts of the changes that may occur in soil pH and soil base cation status as a result of acidic deposition. These soil parameters are particularly important because of the linkage of soils, aluminum chemistry, and surface water acidification. The DDRP Level II models were used to project the status of soil pH and percent base saturation 50 years into the future at current levels of deposition and at other possible levels.

Aggregation of data for these model-based analyses was a paramount concern. Although it is a fairly simple task to enter the appropriate data to run a model on one soil sample or even a pedon it is more difficult to combine the chemistry from several thousand statistically linked soil samples, or a subset of these, for input into the models in such a way that the data effectively represent real physical systems. The hazard is that a computerized or batch method of combining or aggregating these data may surreptitiously mask important associations or preferentially weight unimportant associations. The problem faced by DDRP researchers was how to aggregate the data prior to running these models. If the models were run on individual or partially aggregated samples, the problem then, would be how to aggregate the model results. Another strongly linked issue was how to test and select the most appropriate aggregation procedure from a number of approaches. This chapter discusses aggregation approaches that could have been used in the Level II base cation analyses.

### 5.2 BACKGROUND

Base cations are essential for preventing or delaying the acidification of surface waters. In any watershed, there can be several sources of base cations, including the weathering of primary minerals, the cation exchange complex, biological cycling, wind-blown soil materials, and wet and dry deposition. With respect to acidic deposition effects, the most important short-term source of base cations may be the cation exchange complex. Exchangeable cations represent the most labile form of base cations. Consequently, exchangeable base cations are the most significant form of base cations available for the short-term amelioration of acidic inputs.

The exchangeable cation pool is finite. Primary minerals represent, however, an extensive reserve of base cations. The rate of base cation supply or resupply by primary minerals is limited by the rate of mineral weathering. If the rate of removal exceeds the rate of supply, affected watersheds

will lose their ability to neutralize acidity and either acute or chronic acidification of soils and surface waters is likely to occur.

The models used in the DDRP Level II base cation analysis consider soil pH and base saturation and provide two independent algorithms to simulate exchange processes in soils. The two models were formulated by Reuss and Johnson (1985) and Bloom and Grigal (1985). In general, these models consider soils in isolation of other watershed processes. The Bloom-Grigal model is a one-box (i.e., one aggregate horizon) model. The Reuss-Johnson model is an n-box (i.e., multiple horizons) model based on soil chemical first principles. The Bloom-Grigal model is a mixture of first principles and empirical relations.

For interim assessments and model testing exercises, simplistic aggregation methods were used. Soil chemical data were weighted by horizon and pedon thickness to obtain aggregated values at the sampling class level. These values, then, were weighted by the areal extent of the respective sampling classes on the watershed and combined to provide one aggregated value per watershed for input into the models. The common approach (Section 3.3.2) represents a modification of this aggregation procedure. The common approach can be compared to the aggregation approaches discussed in the following subsections.

## 5.3 SPECIFIC AGGREGATION APPROACHES FOR THE LEVEL II BASE CATION SUPPLY ANALYSES

### 5.3.1 Aggregation Approach

Because soil chemistry can be markedly different between soil horizons, simple averaging and thickness weighting prior to input to the models can result in the loss of important chemical information. The principal aggregation approach used in the base cation analysis aggregates soil chemical data to sample class within master horizons (e.g., O, A+E, B, C; notice that B/C horizons have been treated as B horizons and A/B horizons as A horizons) prior to running the models. The aggregation to the within-sample-class master horizon level and to the watershed master horizon could be computed the same as in the common approach (Section 3.3.2). The model results would then be aggregated or combined to describe the model predictions at the watershed level. A forecast can be made for each master horizon so that different hydrologic routing scenarios can also be considered.

In addition to soil chemical data, the models require information about acidic deposition. For the Level II base cation analysis, volume-weighted annual average precipitation amounts and

compositions were required for each watershed, along with estimates of dry deposition and evapotranspiration.

### 5.3.2 Aggregation of Model Results

The final step in the base cation aggregation plan was the combining of master horizon model results to weight the model forecasts on a watershed basis. The model results can be multiplied by the respective mean master horizon thickness, summed across master horizons, and divided by the sum of the mean thicknesses. The result is one aggregated value per watershed.

## 5.4 EVALUATION OF AGGREGATION SCHEMES

Aggregation approaches can be compared using both parametric and nonparametric procedures. Parametric procedures include regression analyses to compare the slopes of constituent concentrations through time to detect differences among aggregation approaches. Nonparametric approaches, such as the seasonal Kendall tau test, also can be used to test for differences in slopes among aggregation procedures. Differences among aggregation procedures do not indicate which approach would produce accurate 50-year forecasts but they do indicate the uncertainty in forecasts contributed through aggregation.

This aggregation plan was intended to minimize the amount of aggregating done prior to running the Level II models and, at the same time, maximize the amount of discrete soil chemical information that could be used in the models. This approach allows the models to more effectively describe the effect of acidic deposition on watershed soils.

# SECTION 6
# AGGREGATION FOR SULFATE ADSORPTION ANALYSES

## 6.1 PROBLEM STATEMENT

The primary objective of Level II sulfate analysis was to determine the response time (principally time to sulfate steady state) for sulfur in DDRP watersheds, in order to assess the extent to which sulfate adsorption is acting as a delayed response process in the NE, M-APP, or SBRP. Results from these analyses were used with results from other DDRP data analyses to classify the response times of individual watersheds.

The concern with data discussed in this chapter applies principally to single factor (Level II) analyses of sulfate retention. Although the principal use for aggregated data discussed in this chapter is the Level II sulfate analysis, data derived in this exercise were used directly in the Level III models, and the derived isotherm data were used in the Level I correlation analyses with surface water sulfate and other watershed data (Chapter 4).

Two primary types of variables are considered in this chapter: (1) equilibrium soil solution sulfate (ESSS), which estimates soil solution sulfate concentration (for comparison to surface water sulfate concentration), and (2) coefficients for sulfate adsorption isotherms, which describe the partitioning of sulfate between adsorbed and dissolved phases within the soil and are used to predict changes in sulfate mobility with time. Both variables are derived from adsorption isotherms determined in DDRP for individual soils, but there are significant differences in the aggregation procedures used to generate watershed values for the two variables. In both cases, however, aggregation was based on the common approach outlined in Section 3.3. Soil solution sulfate (ESSS) is an intensity variable controlled in the soil by kinetically rapid sorption processes, so its value is determined principally by equilibrium with the last soil in contact with the water. Aggregation thus focuses on the soil horizon(s) believed to have the final contact with soil water before it leaves the soil. The second set of variables in this analysis, the isotherm data used to predict changes in adsorbed sulfate and in surface water sulfate, represents capacity factors, so all soil horizons can be included in the aggregation process. The aggregation procedures are described in Section 6.3. In conjunction with the Level I analyses, ESSS was also computed for all DDRP watersheds for comparison to surface water chemistry variables.

## 6.2 BACKGROUND

The role and importance of sulfate in the acidification of surface waters has been widely studied and reported. In most areas receiving acidic deposition, sulfate is the principal anion in deposition, and cation leaching from soils by sulfate is considered the principal driving mechanism for surface

water acidification. Within terrestrial systems, sulfate either can be retained in a watershed or can pass through soils and act as a mobile anion or "carrier" counterion for basic/acidic cations in runoff to surface waters. In many geographic regions receiving acidic deposition, such as the Northeast and Upper Midwest in the United States and the Scandinavian countries, sulfate retention in most watersheds is typically very low. Watershed sulfur input/output budgets in the majority of catchments are balanced, so that surface water sulfate concentrations and the extent of cation leaching/ acidification are controlled by deposition inputs. In other regions, most notably the southeastern United States, a significant fraction of incoming sulfur is retained in the watershed, principally by sulfate adsorption in soils. To the extent that sulfate is retained in the watershed, cation leaching and potential acidification are prevented or at least delayed.

### 6.2.1 Underlying Assumptions and Approximations

In the design of the DDRP, there was an explicit assumption that adsorption by soils is the only process significantly influencing net sulfate mobility through watersheds. Other processes are actively involved in soil sulfur cycling, including S transformations from inorganic to organic states, biotic uptake, and sulfate reduction. For most such processes, however, the net effect on sulfur budgets in DDRP watersheds is estimated to be small [e.g., biomass accretion (Likens et al. 1977; Johnson et al. 1982) and in-lake reduction (Shaffer et al., 1988; Shaffer and Church, 1989)]. In the case of soil organic matter, the rate of sulfur uptake is large, but turnover is also rapid, with the end result that net accumulation in soil organic pools is apparently small (Fuller et al. 1986; sulfur budget data of Rochelle and Church, 1987). In contrast, field and laboratory data provide strong evidence that sorption serves as a control (buffer) and as a net sink for sulfate in many soils.

In developing chemical models and aggregation schemes for the sulfate analyses described here, a set of assumptions/approximations were made to define soil-water interaction. Based on the assumption that sorption is the sole process controlling sulfate mobility, and that sorption is a kinetically fast process we assumed phase equilibrium in all cases. This means that the effect of a particular soil on sulfate mobility is determined by occurrence of soil-water contact, rather than by contact time. A second, more problematic issue was to define hydrologic pathways. One approach would have been to assume complete soil contact for all water, i.e., that there is no lateral flow from upper soil horizons due to preferred channel flow (macropores) or occurrence of impermeable horizons. Alternatively, recognizing that macropore flow and lateral flow do occur, we could have estimated the fraction of flow by those paths and incorporated it explicitly into the models. A third approach would have been to identify or define a surrogate for such flow (e.g., a porosity or texture variable, SCS hydrologic group) and incorporate it into aggregation as a soil weighting factor. For actual analyses, no objective basis was identified for estimating the extent of lateral or macropore flow, so no aggregations for alternate flow routing were conducted.

The common aggregation approach (Section 3.3.2) could be modified by weighting by a surrogate variable, such as the SCS hydrologic group, to represent preferred/lateral flowpaths (Section 3.3.1.1). For intensity variables, a third approach would be to compare aggregation using the entire watershed with aggregation for only a buffer strip adjacent to the lake or stream (Section 3.3.1.2). For capacity variables, the entire watershed is assumed to play a role in the supply and retention of ions, so all aggregations for capacity variables (including isotherm variables to predict time to sulfate steady state) are at the whole-catchment scale. Regression analysis could be used to compare the results of several aggregation procedures with related surface water parameters (e.g., ESSS with lake or stream sulfate, sum of base cations with ANC) to determine the aggregation approaches most strongly related to surface water chemistry. Selection of the most appropriate approach using regression analysis is not feasible for capacity variables, because there is no dependent variable for comparison (i.e., we do not have a true value of time to steady state for sulfate). Evaluation of results from the various aggregation approaches for intensity variables, however, can provide useful guidelines for deciding whether to include hydrologic weighting in the aggregation for sulfate-related capacity variables.

### 6.2.2 Data Used for Aggregation

The initial activity in Level II sulfate analysis was the generation of adsorption isotherm data for sulfate in soils of the DDRP watersheds. Adsorption isotherms (Figure 6-1) describe the partitioning of sulfate between dissolved and adsorbed phases for individual soils, and can be used with appropriate hydrologic and deposition data to predict temporal changes in soil sulfate pools and in solution as sulfate is added to the soil column. For each DDRP soil, isotherms were determined by equilibrating a set of soil-water slurries containing different amounts of added sulfate; six such slurries, with initial dissolved $SO_4$ concentrations ranging from 0 to 2000 $\mu$eq $SO_4$/L, were used for each soil. Using a nonlinear least squares routine, data for individual soils were fitted to an extended Langmuir equation of the form:

$$E_c = \frac{C * B_1}{C + hfsat} + Y_{int} \qquad \text{(Equation 6-1)}$$

where:
- $C$ = dissolved sulfate ($\mu$eq/L)
- $E_c$ = net adsorbed $SO_4$ at C (meq/kg)
- $E_{max}$ = sulfate adsorption capacity ($E_c$ at infinite C) (meq/kg)
- $B_1$ = $E_{max}$ - $Y_{int}$ (meq/kg)
- hfsat = dissolved $SO_4$ at $E_c$ = 1/2 $B_1$ - $Y_{int}$ ($\mu$eq/L)
- $Y_{int}$ = Y-intercept of fitted line (meq/kg)

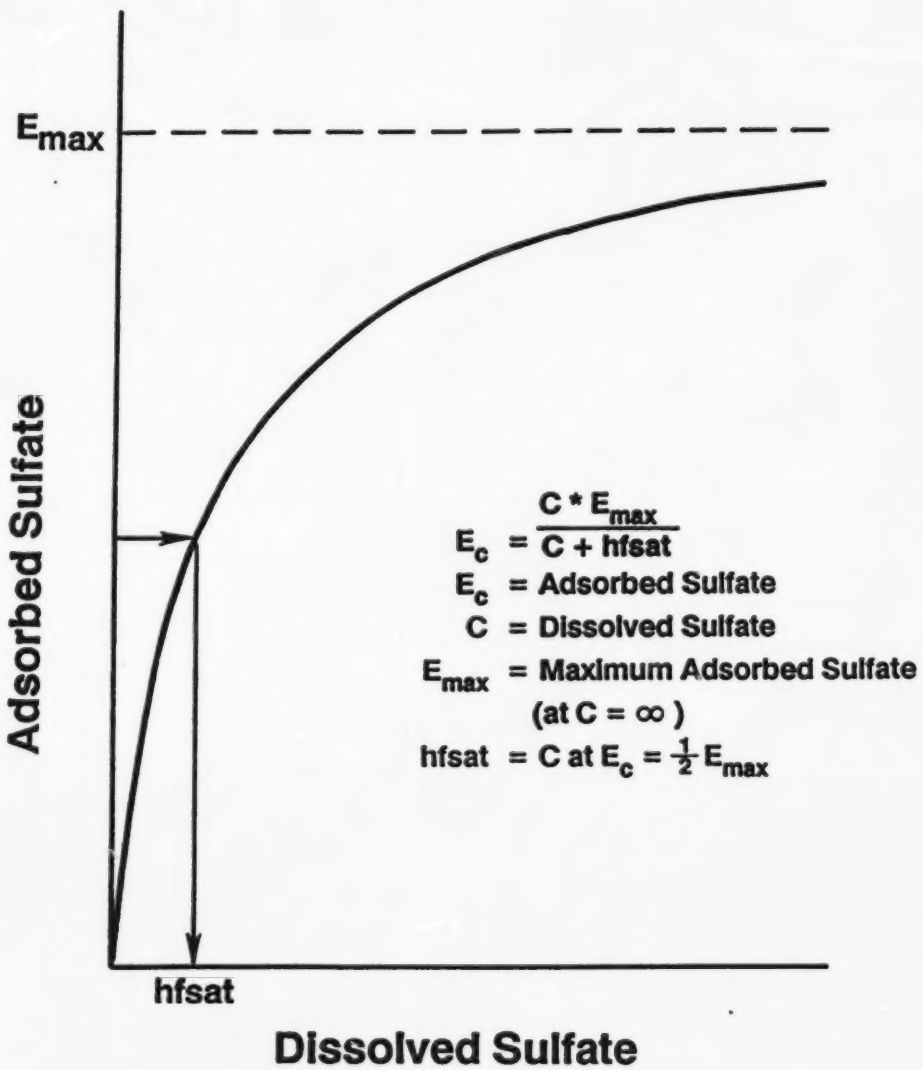


Figure 6-1. Adsorption isotherms for partitioning of sulfate between dissolved and adsorbed phases. Note that $E_{max} = B_1$ when the line passes through the origin.

The extended form of the Langmuir equation used here (Figure 6-1) incorporates the sorption dynamics of both added sulfate and native sulfate (i.e., $SO_4$ already present on soils at the time of collection). In using this equation, we compute net adsorption of sulfate on soils. $Y_{int}$ (actually, $-Y_{int}$) estimates the native sulfate pool active in sorption equilibrium. Using the extended form of the equation, the X-intercept is equal to, and in fact defines, ESSS. For an individual soil, this value represents the dissolved sulfate concentration at which a soil is predicted to neither adsorb nor desorb sulfate, and thus serves as an estimate of sulfate concentration for water in, or flowing from, that soil. To compute time to steady state for sulfur, the three variables that define the isotherm equation for each soil ($B_1$, hfsat, and $Y_{int}$) were indirectly aggregated as described in Section 6.3.1 and used in a dynamic model.

## 6.3 SPECIFIC AGGREGATION APPROACHES FOR SULFATE ADSORPTION ANALYSES

The basis of aggregation for sulfate parameters was the common approach described in Section 3.3.2.

### 6.3.1 Equilibrium Soil Solution Sulfate

Using the isotherm data described above, the first aggregation objective was to determine watershed values of ESSS, then to determine the relationship between ESSS and surface water sulfate concentrations. Values of ESSS, aggregated to watershed values, can be compared to surface water sulfate concentrations using simple regression analyses. If adsorption does control surface water sulfate, and if data are properly aggregated, there should be a high correlation between sulfate concentrations in soil solution and surface waters of a watershed. High correlations between ESSS and lake or stream sulfate do not prove that adsorption by soils controls surface water sulfate, but low correlations would suggest that:

1. aggregation has been done inappropriately;
2. some other process actually controls surface water sulfate; and/or
3. batch isotherm data do not effectively (even in a qualitative sense) describe sulfate partitioning under field conditions.

An inability to obtain a high correlation for any of the proposed aggregation schemes could be interpreted as suggesting the second or third alternative, and would call into question the underlying premises of Level II sulfate analyses.

The common aggregation approach could be modified by aggregating data from sample class/horizon values to a watershed value, using area weighting (% of total watershed area covered by each sample class) and either (1) weighting factors for each sample class/horizon based on SCS

hydrologic class and determined through empirical fitting using selected soil-surface water chemistry pairs or (2) equal weighting factors (other than area) for all sample classes and horizons.

This aggregation step could be done for two areas in each DDRP watershed. First, it could be done using the entire watershed. Second, it could be done using a buffer strip around the perimeter of each lake or stream. Elevational buffers, all areas from 0 - 40 ft above lake elevation, could also be used to delineate hydrologically important catchment areas. An alternative to using all major soil horizons would be to use only a single horizon, either the B or bottom (B or in most cases, C) horizon. This is a special case of the common approach, with a weighting factor of 1.0 for the indicated horizon and a factor of 0 for other horizons. This approach is justified by the assumption that the "last" horizon seen by soil water controls its final solution chemistry, therefore only that final chemically active soil horizon needs to be identified and considered. This approach could be evaluated for sulfate along with the common approach used for all soils, and might be preferable to one of the common approaches if it provides a significant improvement in correlation of ESSS with surface water sulfate.

### 6.3.2 Predicted Time to Sulfate Steady State

The second use of isotherm data, predicting time to steady state for sulfate, represents the focal point of Level II sulfate analysis, which was to predict watershed response to continued sulfur deposition at current or altered loadings. To generate time predictions of sulfate mobility, a modified subroutine of the MAGIC model (Cosby et al., 1985a,b) was used. The subroutine was an equilibrium, mass-balance model with sulfate mobility described by a Langmuir or extended Langmuir isotherm. The model uses a soil described by 1 - 10 horizons; initial soil properties and adsorption characteristics are input variables, along with deposition, precipitation, and runoff. Soil horizons are treated as a series of continuously stirred tank reactors, with phase equilibrium assumed in each horizon. Flow was routed sequentially through each horizon in actual model runs, although hydrologic weighting could have been used during aggregation, if there had been an objective basis for estimating hydrologic routing coefficients for aggregation. The model was run using one-year time steps and long-term average rainfall and runoff, along with historic estimates of emissions (Gschwandtner et al., 1985), scaled to current deposition, and with various future deposition scenarios.

In generating aggregated watershed isotherms for use in the MAGIC model, the first consideration was to decide which variable(s) to aggregate to effectively describe soil-solution sulfate partitioning. In aggregating isotherm data, the important consideration is to describe the partitioning of sulfate (the instantaneous slope of an isotherm) over a dissolved $SO_4$ concentration range of ca 0 - 300 $\mu$eq/L, i.e., from historic to future steady-state concentrations in surface waters. One approach to

the first aggregation step, which goes from individual soils to an aggregation group (all soils from a particular horizon for all pedons in a sample class), was to simply pool the raw isotherm data points (6 per soil) for all soils in an aggregation group and fit a single isotherm to all points. This approach was tried (using partial, raw DDRP data) and abandoned, because there is substantial variability among points and a preponderance of points at low dissolved sulfate, resulting in an aggregate isotherm that was often nearly linear, with an x-intercept and slope unlike (usually lower than) most individual soils. A second approach, fitting isotherms to individual soils and then aggregating derived isotherm coefficients ($B_1$, $Y_{int}$, and the half-saturation constant), was also tried and rejected, because of variability and interdependence among the three isotherm coefficients, which resulted in unrepresentative aggregate isotherms (Shaffer and Stevens, 1990). Most values of hlfsat and $B_1$ for a given aggregation group fall within a fairly narrow range, but for some soils the fitted isotherms are nearly linear and values of those coefficients are orders of magnitude higher than for other soils in the aggregation group. If only one of the isotherm coefficients varies among soils in a group, aggregation on that variable would be the preferred means of aggregation, but in reality all three coefficients can vary widely and interdependently.

The method used was to fit isotherms for individual soils in an aggregation group, then to compute the values of $E_c$ (Equation 6-1) corresponding to specific concentrations of C (dissolved sulfate) (i.e., C=0, 25, 50, 100, 200,...2000 meq/L), based on the equation of the fitted isotherm. Using data from all samples in that group, a mass-weighted average value of $E_c$ corresponding to each value of C was computed. A new isotherm was fitted to these aggregate points, yielding a single isotherm to represent the aggregation group. A similar procedure was used for each step of the aggregation (individual soil to master horizon within pedon; pedon/horizon to sample class/horizon; and sample class/horizon to watershed horizon). The procedures are described in the following paragraphs.

Aggregation procedures for isotherm data that can be used with the MAGIC model are relatively straightforward; as with ESSS, aggregation can be done by first going from individual soil to sample class (within master horizons), then from sample class to watershed. Because the MAGIC submodel works with individual soil horizons in a composite pedon, vertical aggregation is effectively done by the model and no vertical aggregation of data is needed (except for collapsing subhorizons to major soil horizons in an initial aggregation step). For extrapoloratory analyses, data were collapsed to values for one (A+E+B+C) or two (A/E/B,C) horizons, but for routine applications, data were aggregated to three mineral horizons (A/E,B,C horizons). Notice again that isotherm data represent

capacity variables, so that all aggregations for isotherms were done using mass weighting of the data. Specific steps in the aggregation of isotherm data include:

1. Determine (fit) isotherms for individual soils, using a nonlinear fit routine with an extended Langmuir equation; compute values of adsorbed sulfate corresponding to C= 0, 25, 50, 100,...,2000 $\mu$eq/L.
2. For all soils in each aggregation group, calculate a mass-weighted average of $E_c$ corresponding to each value of C.
3. For the derived (C, $E_c$) data pairs for each aggregation group, fit a new nonlinear isotherm; this curve represents the aggregate isotherm for that aggregation group (i.e., pedon/master horizon).
4. Repeat steps 1 to 3 to aggregate data from pedon/horizon to sample class/horizon.
5. Go from sample class to watershed (for each major horizon), repeating steps 1 to 3 except:
   a. using the aggregated isotherms from step 4; and
   b. including the area (of each sample class on a watershed) as a weighting factor, resulting in weighting by: area * mass per unit area.

This procedure was rigorously evaluated for DDRP soils in the SBRP, and was found to be very effective as a means of representing the slopes of individual isotherms (Shaffer and Stevens, 1990). The isotherms generated by this procedure represent aggregate isotherms for each major soil horizon for the watershed, and as noted earlier, were used directly in the MAGIC model without additional vertical aggregation. This procedure can be done with or without hydrologic weighting factors, based upon their apparent significance in aggregations for intensity variables.

An alternative aggregation approach was assessed for a subset of DDRP watersheds, which involved running the MAGIC model with data from individual soil pedons (using deposition, precipitation, and runoff data for the watershed being modelled, not the watershed on which that pedon was located), then aggregating the response functions of the model. Response vectors for individual pedons can be arithmetically averaged to the sample class level, then the aggregate sample class responses can be aggregated using area-weighting to provide a single watershed response forecast. Inasmuch as precipitation, deposition, and runoff (and thus predicted sulfate response of the soil solution) vary by watershed, a principal disadvantage of this approach was that the response of each pedon had to be forecast for every watershed on which the sample class for that pedon occurs.

## 6.4 EVALUATION OF AGGREGATION SCHEMES

One of the potential concerns in aggregating and evaluating isotherm data is that there is no direct means of assessing the quality of the aggregated isotherm data. Actual times to future sulfate steady state are obviously unknown, and there are no other watershed variables that can be meaningfully compared to the isotherm coefficients. For a few watersheds with sufficient monitoring records (mostly in the Southern Blue Ridge), predicted rates of change for $SO_4$ (based on aggregated isotherm data) were compared to measured rates of change for sulfate in surface waters. In addition, for watersheds not at steady state, we compared uncalibrated model predictions (based on isotherm data and other variables with high uncertainty, such as historic sulfur deposition) for 1984-85 to measured NSWS sulfate concentrations in those years. Although these comparisons cannot provide a quantitative evaluation of the isotherm aggregation procedure or of the aggregated data, they provide a check against gross errors and an intuitive basis for assessing the effects of aggregated data on forecast watershed response time to sulfate steady state. Results described in Section 9.2 of Church et al. (1990) show that the common aggregation approach provided aggregate values of ESSS, model predictions of sulfate for the modelling base year [(1984 (NE); 1985 (SBRP)], and rates of change for surface waters that compare well to observed values.

## SECTION 7
## AGGREGATION FOR DYNAMIC WATERSHED MODELING

### 7.1 PROBLEM STATEMENT

The DDRP Level III analyses used dynamic watershed models to forecast the response of 145 NE, 37 M-APP, and 35 SBRP watersheds to varying levels of acidic deposition over the next 50 years. Three watershed models with varying levels of spatial and temporal resolution were used in the DDRP Level III analyses: Enhanced Trickle-Down (ETD), Integrated Lake-Watershed Acidification Study (ILWAS), and Model of Acidification of Groundwater in Catchments (MAGIC).

These three models incorporate the various processes considered important in controlling surface water acidification, such as watershed hydrology, sulfate adsorption, ion exchange, and mineral weathering but at different levels of spatial and temporal resolution. Major differences among the three models are related to the spatial-temporal characterization of the watershed, which results in each model having unique advantages and limitations. Regardless of the model, however, the aggregation procedure used to characterize the watershed must reflect the spatial-temporal watershed attributes influencing surface water chemistry for satisfactory model predictions or forecasts. It is important, therefore, to determine if the aggregation procedure influences the long-term predictions or forecasts.

Several questions related specifically to aggregation and watershed modeling are:

1. Are there any underlying principles related to watershed aggregation for dynamic models?
2. Does the aggregation scheme significantly influence long-term forecasts?
3. Is there an aggregation approach that is most appropriate for long-term forecasts?

The specific objectives for Level III aggregation analyses were:

1. to develop a general protocol related to watershed aggregation for watershed models based on model structure and first principles;
2. to evaluate the effects of varying aggregation approaches on long-term model forecasts for each of the three DDRP models; and
3. to select the most appropriate aggregation strategy for each of the three models to be used in DDRP based on theoretical and pragmatic considerations.

## 7.2 BACKGROUND

### 7.2.1 Previous Approaches

The effect of the aggregation procedure on model predictions or forecasts, in general, has not received adequate attention. The effect of spatial variability and aggregation of hydrologic response units within a watershed on the simulation of overland and channel flow was evaluated by Shanholtz et al. (1981). In general, Shanholtz et al. (1981) found that the prediction error increased as the level of aggregation decreased (i.e., increased fine-scale spatial resolution in the watershed). Loague and Freeze (1985) also observed that prediction uncertainty increased as fine scale resolution in how processes were represented in the model increased. Spatial variability in the watershed becomes increasingly important as the model scale of resolution becomes finer. Wosten et al. (1985) obtained basic soil physical data (e.g., grain size, texture, bulk density, water retention, hydraulic conductivity) from a detailed soil survey, compared horizons, developed characteristic distributions, and used these characteristic parameter distributions in a regional soil water simulation model. This aggregation approach resulted in good agreement between predicted versus observed evapotranspiration estimates.

Theoretical studies of the influence of aggregation on mathematical model simulation uncertainty have been conducted by several authors. O'Neill and Rust (1979) evaluated the effect of potential aggregation error or uncertainty in a theoretical ecological model and provided several simple rules for minimizing aggregation error. These rules included lumping components with similar turnover times and lumping rare species with common species. As noted in Section 3.2, Gardner et al. (1982) expanded on these analyses and provided several pragmatic rules for aggregation. Luckyanov (1983) and Luckyanov et al. (1983) focused on the theoretical aspects of aggregation and formulated a general theorem for linear aggregation and linear separability in linear models. This general theorem, unfortunately, is not applicable to any of the DDRP models. Most ecosystem models are either explicitly or implicitly nonlinear.

### 7.2.2 Characteristic Time and Length Scales

Regardless of the nature of the process, all processes must be simplified and/or aggregated to be represented in mathematical notation. Whether explicitly or implicitly formulated, this reduction or simplification results in a representation only of a subset of the entire process range.

The resulting subset is necessarily constrained by time and length scales characteristic of the processes being represented. Time, space, and the interaction of these two scales is an important concept that had to be developed both for DDRP and for the ecological modeling community. Time and length scale analyses can be used to identify and formulate appropriate aggregation procedures.

Characteristic length scales are well established in the area of fluid mechanics and other engineering disciplines. In general, any hydrodynamic equation or study that incorporates turbulence has a length (and time) scale that characterizes its applicability. Erroneous results are possible if these equations are applied outside their characteristic ranges.

Characteristic time scales also are implicitly included in all mathematical formulations. The characterization or conceptualization of any process, such as time of concentration of stormflow, constrains the applicability, validity, and realization of predictions from this formulation.

Many processes conceptualized on a fine-time scale (i.e., seconds to hours) cannot simply be integrated over time to describe daily or seasonal processes, because the driving variables or forcing functions are usually quite different at grossly different time scales. An example of the relation between time-length scales for various hydrologic processes can be illustrated by considering the factors required to predict mean annual discharge, average seasonal discharge, and a storm hydrograph. Mean annual discharge can be reasonably predicted with an estimate of the watershed area and the mean annual precipitation over the basin. Fine scale processes are imbedded in larger scale factors and do not have to be considered. Evapotranspiration, for example, is implicitly incorporated in the mean annual runoff at an annual time scale. For an estimate of average seasonal discharge, however, evapotranspiration becomes an important process to consider, particularly during the growing season. The spatial scale for precipitation now is the catchment within the basin. To predict a storm hydrograph, both the magnitude and duration of precipitation is required on at least an hourly basis and at the subcatchment spatial scale. Processes related to soil moisture (antecedent conditions), vegetative cover (interception estimates), and subsurface flow become important. An example of the interaction between time and length scales for a biological process is illustrated in Figure 7-1.

Determination of the effects of different aggregation procedures on the long-term forecasts from the three models applied in DDRP was initiated in the DDRP and will be formalized in the Watershed Manipulation Project (WMP). The WMP is designed to test and evaluate the behavior of the DDRP models through field chemical manipulations.

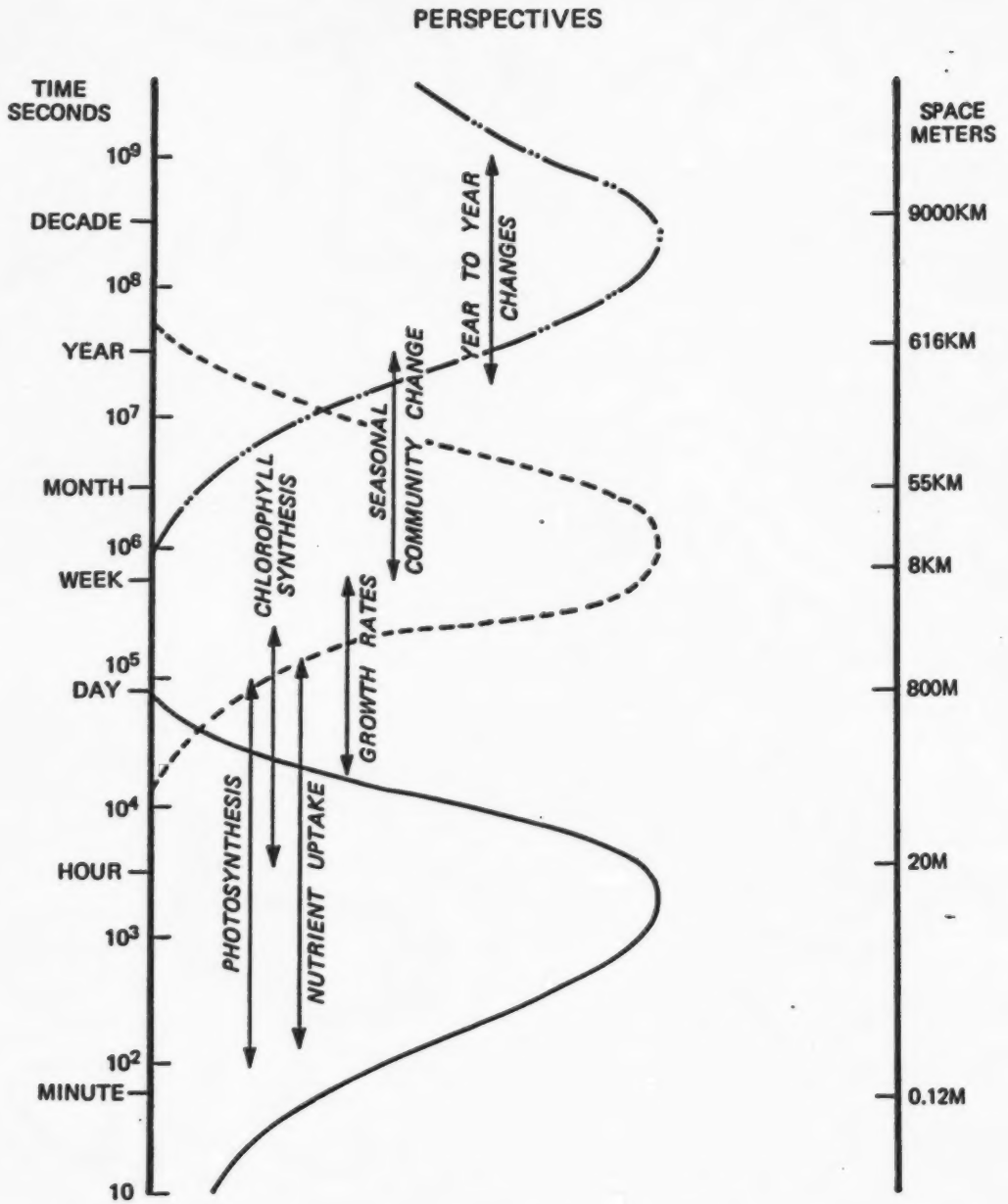


Figure 7-1. Interaction of time and length scales with respect to important processes in the algal community (after Harris 1980).

## 7.3 SPECIFIC AGGREGATION APPROACHES FOR DYNAMIC WATERSHED MODELING

The three models used in the DDRP Level III analyses represent the spatial watershed characteristics quite differently. MAGIC has two compartments to represent the soil column and assumes the watershed is horizontally and vertically homogeneous within the soil compartment. ETD has three compartments to represent the soil column and also assumes the watershed is horizontally and vertically homogeneous within the soil compartments. ILWAS represents each horizon in the soil column and divides the watershed into subcatchments. The soils are assumed to be horizontally and vertically homogeneous within these specific compartments.

The three models also have different simulation time scales. The time scale for the MAGIC model is annual. MAGIC was specifically formulated for long-term forecasts. The time scale for the ETD and ILWAS models is daily to weekly. These models were formulated for seasonal and annual forecasts. The aggregation procedures for each model, therefore, were model specific. The specific approach for analysis of the aggregation scheme was to compare and contrast the general procedures currently used by the model developers with the approach suggested by the time-length scale analysis and the common approach identified in Chapter 3 for all levels of analysis. These different aggregation procedures were compared using long-term forecasts of system response to acidic deposition from both a lake and stream watershed.

## 7.4 EVALUATION OF AGGREGATION SCHEMES

The general approach for evaluating the aggregation procedure was as follows:

1. Describe the aggregation procedures used for the DDRP model calibration and obtain data sets from the three modeling groups.
2. Propose an aggregation procedure based on a time-length scale evaluation of each model and prepare aggregated data sets.
3. Provide the data set prepared by the generic aggregation approach discussed in Section 3.3.2.
4. Compare these three aggregation procedures (if they differ) including a 50-year forecast using the aggregation procedures for two watersheds: a lake (Clear Pond) and a stream watershed (Coweeta Watershed No. 36).
5. Using paired comparison tests, determine if there are significant differences among the 50-year forecast constituent concentrations as a function of the aggregation scheme.
6. Assess the potential effect of different aggregation approaches on regional estimates of watershed response.
7. Recommend an aggregation procedure for each model.

### 7.4.1 Time-Length Approach

Time and length scale evaluations were conducted on the three DDRP models emphasizing those processes and process interactions expected to influence long-term acidification of surface water chemistry (i.e., those processes discussed in previous chapters). The specific aggregation procedure used with any particular model had to provide representative watershed values for model parameterization and calibration that reflect the time-length scales for the process interactions incorporated in that model structure.

An approach similar to Ford and Thornton (1979), which considers both theoretical and pragmatic constraints in estimating applicable time-length scales, was used to evaluate appropriate aggregation procedures for the three DDRP models.

The time and length scale analyses focused on the watershed and the processes of importance at this spatial scale. The time scale associated with this spatial scale is dependent on the hydrometeorological forcing functions. There is an interaction, however, between space and time in determining the appropriate spatial-temporal scale. An example of the interaction between time and length scales and process aggregation is shown in Figure 7-1. A similar figure was developed to represent various watershed processes, showing the increased aggregation of watershed processes as the temporal-spatial scale increases. Scale problems represent one of the major factors that needs to be clearly identified in this section. The forcing functions for the watershed are the hydrometeorological inputs. Spectral analysis was evaluated based on the power associated with different temporal-spatial scales.

A desirable spatial-temporal scale for hydrologic modeling, for example, corresponds with a trough or low power portion of the power spectrum curve for precipitation (Figure 7-2). The integration of these factors with the model structure represents the appropriate time-length scale and the aggregation protocol for each model.

### 7.4.2 Common Approach

The generic aggregation approach discussed in Chapter 3.3.2 can be used to prepare a third data set for each of the three models.

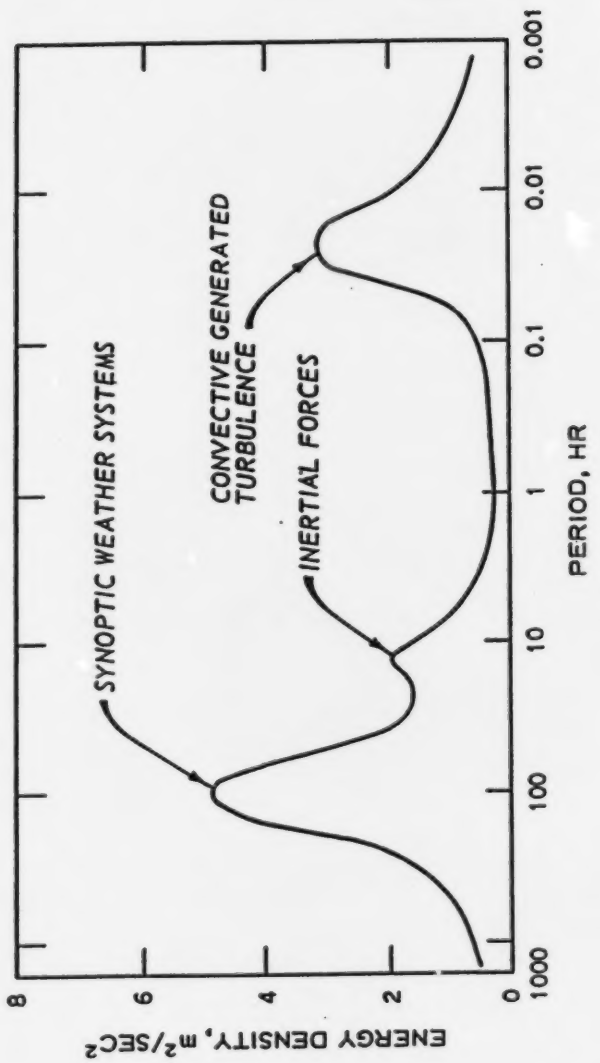


Figure 7-2. Power spectral analysis illustrating three important periods in meteorological data.

### 7.4.3 Comparison

The three models were calibrated on Clear Pond and Coweeta Watershed No. 36 using the three aggregation schemes (if different) followed by 50-year forecasts on each system. These three forecasts were compared, based on surface water chemistry responses, to determine whether different aggregation approaches result in different forecasts. Six chemical constituents, ANC, pH, $SO_4$, Cl, Ca, and Mg, were monitored, because of their significance for surface water acidification. These forecasts were also compared for soil-water chemistry concentrations to determine if the three aggregation approaches result in different soil-solution chemistries. Specific soil-water chemical constituents include pH, $SO_4$, and percent base saturation.

The DDRP considers changes in the volume-weighted average annual constituent values to represent the watershed response to acidic deposition. Two apprcaches can be used to compare the three aggregation procedures. The first approach is parametric regression analysis to determine if the slopes of the constituent concentrations through time are significantly different from each other. The second approach is to use the nonparametric Seasonal Kendall-tau test modified to include multiple comparisons of systems through time. The modified Seasonal Kendall-tau procedure also tests for significant differences in slope through time. This approach has been used successfully in other projects (Payne et al. 1987).

# SECTION 8
# AGGREGATION AND DDRP

## 8.1 INTRODUCTION

The most appropriate procedure for aggregating data is a basic issue for any analysis, from computing descriptive statistics, to multivariate analyses, to forecasting the watershed response to some environmental perturbation with dynamic models. Aggregation of data was recognized as a component of the DDRP analyses that could significantly influence the results and conclusions of these analyses. The method of aggregation could influence the identification of associations (interactions) among system components or processes and significantly increase the uncertainty in model forecasts of watershed responses to acidic deposition. These two factors, interaction and uncertainty, are briefly discussed.

## 8.2 INTERACTIONS

A major strength of the DDRP is the interaction among the levels of analyses. Level I (multivariate) analyses identify associations between watershed attributes and surface water chemistry. The Level II analyses focus on specific processes thought to control or influence surface water acidification. Multivariate analyses can be used to classify watersheds, based on Level II estimates, and determine whether these associations are stationary over time and/or corroborate hypotheses as to which factors control surface water acidification. The dynamic watershed models integrate the factors and processes considered important in influencing surface water acidification. The use of a common data aggregation approach in all three levels of analysis improves the consistency of the results and reduces the effects of the potential confounding factor of different aggregation procedures.

Comparisons among aggregation procedures and levels of analyses can provide greater opportunity to identify associations among variables and indicate those variables or processes that might influence the watershed response to acidic deposition. These comparisons also indicate areas of uncertainty.

## 8.3 UNCERTAINTY

Uncertainty and error analysis are important components of the DDRP. The uncertainty associated with forecasts 50-years into the future is likely to be large. These forecasts are intended to provide a relative, rather than an absolute, indication of changes in surface water chemistry that might be expected under current and alternative levels of deposition. Two sources of uncertainty, parameter and input error, were evaluated through error analysis on a selected subset of lakes or streams in the respective region. Underlying these sources of error, however, is the potential uncertainty contributed through data aggregation.

If the aggregation approach has a significant effect on the analytical results, then the error bounds on the final results and conclusions might be increased. A primary reason for performing the exercises in this Aggregation Plan is to determine if the approach used to aggregate the data has a significant effect on the results of the subsequent analyses. If the effect of aggregation is limited, its potential influence on the results is not eliminated; it may still be a minor component of error.

### 8.4 DDRP AGGREGATION APPROACHES

For the DDRP, the selection of the appropriate aggregation procedure was based on first principles, underlying assumptions of each aggregation approach, and results from other levels of analysis. The rationale for the aggregation procedure selected was clearly stated, the underlying assumptions identified, and an estimate of variance associated with the approach provided.

## SECTION 9
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